Atomic structure calculations for F-like tungsten

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Energy levels, wavefunction compositions and lifetimes have been computed for all levels of $1s^22s^22p^5$, $1s^22s2p^6$, $1s^22s^22p^43s$, $1s^22s^22p^43p$, and $1s^22s^22p^43d$ configurations in highly charged F-like tungsten ion. The multiconfigurational Dirac–Fock method (MCDF) is adopted to generate the wavefunctions. We have also presented the transition wavelengths, oscillator strengths, transition probabilities, and line strengths for the electric dipole (E1) and magnetic quadrupole (M2) transition from the $1s^22s^22p^5$ ground configuration. We have performed parallel calculations with the flexible atomic code (FAC) for comparing the atomic data. The reliability of present data is assessed by comparison with other theoretical and experimental data available in the literature. Good agreement is found between our results and those obtained using different approaches confirm the quality of our results. Additionally, we have predicted some new atomic data for F-like W that were not available so far and may be important for plasma diagnostic analysis in fusion plasma.

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1. Introduction

Relativistic atomic data on tungsten ions, such as transition wavelengths and transition probabilities are useful in plasma physics particularly due to development of future fusion reactors. Indeed, as sputtering at the surface with plasma contact cannot be avoided completely, tungsten will be an intrinsic impurity in these plasmas. In recent years, highly charged states of tungsten have been studied in tokomaks, laser-produced plasma, and at electron beam ion trap (EBIT).[1–5] Furthermore, highly charged tungsten ions are of interest for atomic theory. With this in mind, we already presented calculations for highly charged tungsten ions,[6,7] and in this paper we reported similar calculations for F-like tungsten.

The atomic data for the F-like W is very limited in the literature. Podpaly *et al.*[8] measured some transitions of the type $^2S_{1/2}$–$^2P_{3/2}$ for F-like W in soft X-ray region using the EBIT (electron beam ion trap). Clementson *et al.*[9] measured transitions from L-shell tungsten ions (including F-like W) using SuperEBIT, employing both crystal and X-ray calorimeter spectrometers. They[9] also identified several additional lines in F-like W. The $2s^22p^{52}P_{3/2}$–$^2P_{3/2}$ magnetic dipole (M1) transition predicted in their work[9] is important for the ITER plasma diagnostics. Feldman *et al.*[10] measured the transition wavelength and intensity for the $2p^43p$ $^4D_{7/2}$–$2p^43p$ $^4F_{9/2}$ transition in F-like W. Also, Putterich *et al.*[11] measured 4 transition lines for $2s^22p^5$–$2p^53d$ transition in F-like W. Beiersdorfer *et al.*[12] observed some transition lines for F-like W using EBIT for $2p^{52}P_{3/2}$–$2p^43l$ transitions. They[12] have also performed calculations using the flexible atomic code (FAC). A detailed compilation of the recent results on spectra of F-like W can be seen in Refs. [13]–[16].

The overall objective of the work described in this paper is to report reliable atomic data for F-like tungsten and compare the calculated values with experimental measurements and other theoretical calculations. As F-like W is highly charged, CI is very important for a reliable determination of energy levels, transition probabilities, and other parameters. For this reason, although our calculations are confined to $1s^22s^22p^5$, $1s^22s2p^6$, $1s^22s^22p^43s$, $1s^22s^22p^43p$, and $1s^22s^22p^43d$ levels, we have included $1s^22s^22p^5$, $1s^22s2p^6$, $1s^22s^22p^43s$, $1s^22s^22p^43p$, $1s^22s^22p^43d$, $1s^22s^22p^44s$, $1s^22s^22p^44p$, $1s^22s^22p^44d$, $1s^22s^22p^44f$, $1s^22s^22p^45s$, $1s^22s^22p^45p$, $1s^22s^22p^45d$, $1s^22s^22p^45f$, $1s^22s2p^53s$, $1s^22s2p^53p$, $1s^22s2p^53d$, $1s^22s2p^54s$, $1s^22s2p^54p$, $1s^22s2p^54d$, $1s^22s2p^54f$, $1s^22p^63s$, $1s^22p^63p$, and $1s^22p^63d$ configurations, as an elaborate CI needs to be included to achieve a better accuracy in the determination of energy levels.

In present calculations, we have used multiconfigurational Dirac–Fock (MCDF) method to generate the wavefunctions. This method was originally developed by Grant *et al.*[17] and revised by many authors.[18–21] We have used the version revised by Norrington[21] which have been successfully applied in many work.[22–25] Further, it is based on jj coupling scheme and also fully relativistic. We have also included the higher order relativistic term which arises from the Breit interaction and quantum electrodynamics (QED) effects (Lamb shift and vacuum polarization). Additionally, we have used the option of EAL (extended average level) in which a weighted trace of the Hamiltonian matrix is minimized which produces a set of orbital describing closely lying state with moderate

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accuracy. This option (EAL) produces comparable results to other options such as AL (average level).

2. Theoretical method

In the MCDF approach, the Dirac–Coulomb Hamiltonian for an N-electron atom or ion can be written as

$$H^{\rm DC} = \sum_{i=1}^{N} H_i + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} |\boldsymbol{r}_i - \boldsymbol{r}_j|^{-1}, \quad (1)$$

where

$$H = c\alpha_i.p_i + \beta c^2 + V_{\rm nuc}(r) \quad (2)$$

is the single-particle Hamiltonian consisting of kinetic energy and its interaction with the nucleus. In Eq. (2), α and β denote 4×4 Dirac matrices, and c represents the speed of light.

The N-electron wavefunction is constructed from central-field Dirac orbitals written as

$$\phi_{nkm} = \frac{1}{r}\begin{pmatrix} P_{nk}(r) & \chi_{km}(\theta,\phi,\sigma) \\ -{\rm i}Q_{nk}(r) & \chi_{km}(\theta,\phi,\sigma) \end{pmatrix}. \quad (3)$$

Here, k is the Dirac angular quantum number, $k = \pm(j+1/2)$ for $l = j\pm 1/2$, so $j = k-1/2$, P_{nk} and Q_{nk} are the radial functions, and m is the projection of the angular momentum j. The two component spin angular momentum $\chi_{km}(\theta,\phi)$ is defined by

$$\chi_{km}(\theta,\phi) = \sum_{\sigma=\pm 1/2} \left\langle lm-\sigma \frac{1}{2}\sigma \middle| l\frac{1}{2}jm \right\rangle {\rm Y}_l^{m-\sigma}(\theta,\phi)\phi^{\sigma}. \quad (4)$$

An atomic state function (ASF) formed for an N-electron system with given total angular momentum J, M, and parity P can be approximated by a linear combination of $n_{\rm c}$ electronic configuration state functions (CSF)

$$|\psi_\alpha(PJM)\rangle = \sum_{i=1}^{n_{\rm c}} C_i(\alpha)|\gamma_i(PJM)\rangle. \quad (5)$$

In Eq. (5), $n_{\rm c}$ is the number of CSFs included in the expansion, $C_i(\alpha)$ are the expansion mixing co-efficients, and α represents all information, such as orbital occupation numbers, coupling, etc. For Dirac–Hamiltonian expectation, we obtain the energy of the N-electron system as

$$\begin{aligned} E_\alpha^{PJM} &= \langle\Psi_\alpha(PJM)|\boldsymbol{H}^{\rm DC}|\Psi_\alpha(PJM)\rangle \\ &= \sum_{ij} C_i^*(\alpha)C_j(\alpha)\langle\gamma_i PJM|\boldsymbol{H}^{\rm DC}|\gamma_j PJM\rangle \\ &= (C_\alpha^{\rm DC})^+ \boldsymbol{H}^{\rm DC} C_\alpha^{\rm DC}. \end{aligned} \quad (6)$$

The Hamiltonian matrix $\boldsymbol{H}^{\rm DC}$ has elements

$$\boldsymbol{H}_{rs}^{\rm DC} = \langle\gamma_r PJM|\boldsymbol{H}^{\rm DC}|\gamma_s PJM\rangle. \quad (7)$$

Requiring Eq. (8) to be stationary with respect to the mixing coefficients leads to the eigenvalue problem to the mixing co-efficients

$$(\boldsymbol{H}^{\rm DC} - E_\alpha^{\rm DC}\boldsymbol{I})\boldsymbol{C}_\alpha^{\rm DC} = 0, \quad (8)$$

where $\boldsymbol{I}$ is the $n_{\rm c}\times n_{\rm c}$ unit matrix. Thus, the atomic energy level E_α^{PJM} can be taken to be eigenvalues of $\boldsymbol{H}^{\rm DC}$.

3. Results and discussion

3.1. Energy levels

We have used different calculation techniques to calculate the energy levels of F-like tungsten, as it is of fundamental interest to atomic theory. These approaches include the multiconfigurational Dirac–Fock (MCDF) method and flexible atomic code (FAC). The FAC is used for two purposes. First, due to lack of much experimental and theoretical work in F-like W, we can compare the results of FAC and MCDF and can show the reliability of our results. Second, in MCDF with our available computational resources, it is not possible to include CI with much larger extent. However, we can perform much larger calculations using FAC and can show the convergence of the results. FAC is also a fully relativistic code[26] and employs the configurational interaction (CI) approach to determine the energy levels and A values. Also, one can perform large calculations within a reasonable time frame using FAC.

In present calculations, the excitation energies (relative to ground state) of the 60 fine-structure levels belonging to the configurations $1s^22s^22p^5$, $1s^22s2p^6$, $1s^22s^22p^43s$, $1s^22s^22p^43p$, and $1s^22s^22p^43d$ have been calculated for F-like W referred to as MCDF as listed in Table 1. For our MCDF calculations, we have used $1s^22s^22p^5$, $1s^22s2p^6$, $1s^22s^22p^43s$, $1s^22s^22p^43p$, $1s^22s^22p^43d$, $1s^22s^22p^44s$, $1s^22s^22p^44p$, $1s^22s^22p^44d$, $1s^22s^22p^44f$, $1s^22s^22p^45s$, $1s^22s^22p^45p$, $1s^22s^22p^45d$, $1s^22s^22p^45f$, $1s^22s2p^53s$, $1s^22s2p^53p$, $1s^22s2p^53d$, $1s^22s2p^54s$, $1s^22s2p^54p$, $1s^22s2p^54d$, $1s^22s2p^54f$, $1s^22p^63s$, $1s^22p^63p$, and $1s^22p^63d$ configurations of F-like W. We have presented the lifetimes of all excited levels in Table 1, which have been reported for the first time for F-like W. Table 1 also reports the wavefunction compositions in both LSJ and JJ coupling scheme for MCDF calculation. In the column "Composition" of Table 1, nl_- denotes $j_- = l-1/2$, while nl corresponds to the $j_+ = l+1/2$. The last column of Table 1 represents the leading percentage of various states. The first number represents the leading percentage of the level corresponding to the level number under the first column then set of numbers of the form $M(N)$. It was verified that jj coupling appears much more adequate than LS coupling, as can be seen from Table 1. The average jj purities were found in range of 70%–100%, while the corresponding LS coupling contributions obtained is very less than jj coupling. In the LSJ notation, CSF are represented only by LS term and seniority of subshell and the final LS term.

We have predicted many new results, which are not available so far. We have presented atomic data for all symmetries of $1s^22s^22p^43s$, $1s^22s^22p^43p$, and $1s^22s^22p^43d$ levels. Also, mixing among some of the relativistic levels is very strong.

Table 1. MCDF energies (in Ryd.), lifetimes (in s), and wave-function compositions of levels in F-like W.

Label	J	Level/Ryd	Lifetime	Composition	
				JJ coupling	*LSJ* Coupling
$2s^22p^5\ ^2P^o$	3/2	0		**100** $2s^22p\text{-}^22p^3$	**100**
$2s^22p^5\ ^2P^o$	1/2	102.0486	4.17×10^{-11}	**100** $2s^22p\text{-}^12p^4$	**100**
$2s2p^6\ \ ^2S$	1/2	137.694	4.51×10^{-14}	**100** $2s2p\text{-}^22p^4$	**100**
$2s^22p^4(^3_2P)3s\ ^4P$	5/2	621.0697	2.61×10^{-14}	**100** $2s^22p\text{-}^22p^2(2)3s$	**68** + **31**(28)
$2s^22p^4(^3_2P)3s\ ^2P$	3/2	621.8796	4.34×10^{-15}	**100** $2s^22p\text{-}^22p^2(2)3s$	**56** + **32**(29)
$2s^22p^4(^1S)3s\ ^2S$	1/2	625.8603	8.76×10^{-15}	**100** $2s^22p\text{-}^22p^2(0)3s$	**65** + **23**(56)
$2s^22p^4(^3_2P)3p\ ^4P$	3/2	631.2407	4.75×10^{-11}	**100** $2s^22p\text{-}^22p^2(2)3p^1$	**31** + **18**(13)+ **16**(33)
$2s^22p^4(^3_2P)3p\ ^2D$	5/2	631.3844	7.44×10^{-11}	**100** $2s^22p\text{-}^22p^2(2)3p^1$	**29** + **26**(38)+ **24**(32)
$2s^22p^4(^1S)3p\ ^2P$	1/2	635.7751	1.25×10^{-11}	**100** $2s^22p\text{-}^22p^2(0)3p^1$	**65** + **19**(57)
$2s^22p^4(^3_2P)3p\ ^4P$	5/2	659.8754	1.19×10^{-12}	**100** $2s^22p\text{-}^22p^2(2)3p^1$	**40** + **26**(8)+ **24**(39)
$2s^22p^4(^3_2P)3p\ ^2S$	1/2	659.9464	1.2×10^{-11}	**100** $2s^22p\text{-}^22p^2(2)3p^1$	**37** + **32**(40)+ **18**(36)
$2s^22p^4(^3_2P)3p\ ^4D$	7/2	659.8753	6.13×10^{-13}	**100** $2s^22p\text{-}^22p^2(2)3p^1$	**67**+**32**(12)
$2s^22p^4(^3_2P)3p\ ^4S$	3/2	663.5196	6.38×10^{-12}	**77** $2s^22p\text{-}^22p^2(2)3p^1$	**24**+**21**(14)
$2s^22p^4(^3_2P)3p\ ^2P$	3/2	665.4188	2.63×10^{-9}	**77** $2s^22p\text{-}^22p^2(0)3p^1$	**50**+**16**(14)
$2s^22p^4(^3_2P)3d\ ^4D$	3/2	670.714	4.36×10^{-14}	**97** $2s^22p\text{-}^22p^2(2)3d^1$	**32** + **23**(42)+ **22**(45)
$2s^22p^4(^3_2P)3d\ ^4D$	5/2	670.885	1.35×10^{-14}	**98** $2s^22p\text{-}^22p^2(2)3d^1$	**35**+**22**(46)
$2s^22p^4(^3_2P)3d\ ^4P$	1/2	671.1567	2.87×10^{-15}	**99** $2s^22p\text{-}^22p^2(2)3d^1$	**50**+**22**(55)
$2s^22p^4(^3_2P)3d\ ^2F$	7/2	670.9401	8.41×10^{-13}	**100** $2s^22p\text{-}^22p^2(2)3d^1$	**34** + **28**(44)+ **28**(48)
$2s^22p^4(^1S)3d\ ^2D$	3/2	675.4067	1.94×10^{-13}	**95** $2s^22p\text{-}^22p^2(0)3d$	**61**+**16**(60)
$2s^22p^4(^3_2P)3d\ ^4D$	7/2	677.3713	9.36×10^{-10}	**100** $2s^22p\text{-}^22p^2(2)3d$	**40** + **27**(53)+ **22**(18)
$2s^22p^4(^3_2P)3d\ ^4F$	9/2	677.4175	7.82×10^{-12}	**100** $2s^22p\text{-}^22p^2(2)3d$	**67**+**32**(51)
$2s^22p^4(^3_2P)3d\ ^2P$	1/2	678.4638	1.27×10^{-15}	**99** $2s^22p\text{-}^22p^2(2)3d$	**50**+**22**(45)
$2s^22p^4(^3_2P)3d\ ^2D$	5/2	680.2594	6.16×10^{-16}	**93** $2s^22p\text{-}^22p^2(2)3d$	**26** + **21**(49)+ **20**(52)
$2s^22p^4(^3_2P)3d\ ^2P$	3/2	680.3573	5.01×10^{-16}	**97** $2s^22p\text{-}^22p^2(2)3d$	**26** + **21**(50)+ **19**(54)
$2s^22p^4(^1S)3d\ ^2D$	5/2	682.9646	9.17×10^{-16}	**94** $2s^22p\text{-}^22p^2(0)3d$	**61**
$2s^22p^4(^3_2P)3s\ ^4P$	3/2	723.6366	4.97×10^{-14}	**98** $2s^22p\text{-}^12p^3(1)3s$	**87**
$2s^22p^4(^3_2P)3s\ ^2P$	1/2	724.3534	1.96×10^{-14}	**100** $2s^22p\text{-}^12p^3(1)3s$	**66**+**33**(56)
$2s^22p^4(^1_2D)3s\ ^2D$	5/2	725.1301	2.41×10^{-14}	**100** $2s^22p\text{-}^12p^3(1)3s$	**68**+**31**(4)
$2s^22p^4(^1_2D)3s\ ^2D$	3/2	725.5919	5.06×10^{-14}	**98** $2s^22p\text{-}^12p^3(2)3s$	**66**+**32**(5)
$2s^22p^4(^3_2P)3p\ ^4P$	1/2	733.4395	2.17×10^{-10}	**100** $2s^22p\text{-}^12p^3(1)3p^1$	**51** + **27**(57)+ **21**(11)
$2s^22p^4(^3_2P)3p\ ^4D$	3/2	733.9161	1.31×10^{-11}	**80** $2s^22p\text{-}^12p^3(1)3p^1$	**56**
$2s^22p^4(^1_2D)3p\ ^2F$	5/2	734.9512	1.51×10^{-10}	**100** $2s^22p\text{-}^12p^3(2)3p^1$	**53**
$2s^22p^4(^1_2D)3p\ ^2P$	3/2	738.0933	1.19×10^{-12}	**79** $2s^22p\text{-}^12p^3(2)3p^1$	**29** + **24**(43)+ **18**(14)
$2s^22p^4(^3_2P)3p\ ^4D$	5/2	762.5287	2.8×10^{-12}	**97** $2s^22p\text{-}^12p^3(1)3p$	**55**+**28**(10)
$2s^22p^4(^3_2P)3p\ ^2D$	3/2	762.8885	7.46×10^{-10}	**86** $2s^22p\text{-}^12p^3(1)3p$	**46**+**24**(7)
$2s^22p^4(^3_2P)3p\ ^2P$	1/2	763.3714	1.61×10^{-14}	**70** $2s^22p\text{-}^12p^3(1)3p$	**23** + **22**(30)+ **19**(11)
$2s^22p^4(^1_2D)3p\ ^2F$	7/2	763.6761	1.47×10^{-9}	**100** $2s^22p\text{-}^12p^3(2)3p$	**67**+**32**(12)
$2s^22p^4(^1_2D)3p\ ^2D$	3/2	764.6281	2.49×10^{-13}	**84** $2s^22p\text{-}^12p^3(2)3p$	**29** + **27**(33)+ **16**(13)
$2s^22p^4(^1_2D)3p\ ^2D$	5/2	764.6376	1.24×10^{-11}	**98** $2s^22p\text{-}^12p^3(2)3p$	**53**
$2s^22p^4(^1_2D)3p\ ^2P$	1/2	768.7536	4.17×10^{-13}	**76** $2s^22p\text{-}^12p^3(2)3p$	**51**+**33**(36)
$2s^22p^4(^3_2P)3d\ ^4D$	1/2	772.7272	6.08×10^{-13}	**93** $2s^22p\text{-}^12p^3(1)3d^1$	**81**
$2s^22p^4(^3_2P)3d\ ^4P$	3/2	773.5953	2.85×10^{-13}	**85** $2s^22p\text{-}^12p^3(1)3d^1$	**37** + **29**(15)+ **16**(24)
$2s^22p^4(^3_2P)3d\ ^4F$	5/2	774.0254	3.0×10^{-15}	**88** $2s^22p\text{-}^12p^3(1)3d^1$	**56** + **17**(23)+ **16**(60)
$2s^22p^4(^1_2D)3d\ ^2G$	7/2	774.5434	1.54×10^{-9}	**100** $2s^22p\text{-}^12p^3(2)3d^1$	**60**+**17**(8)
$2s^22p^4(^1_2D)3d\ ^2S$	1/2	776.1573	7.8×10^{-16}	**89** $2s^22p\text{-}^12p^3(2)3d^1$	**35** + **33**(17)+ **27**(55)
$2s^22p^4(^1_2D)3d\ ^2F$	5/2	776.2118	7.76×10^{-16}	**88** $2s^22p\text{-}^12p^3(2)3d^1$	**45** + **19**(23)+ **17**(16)
$2s^22p^4(^1_2D)3d\ ^2D$	3/2	776.6228	6.89×10^{-16}	**83** $2s^22p\text{-}^12p^3(2)3d^1$	**33** + **24**(50)+ **21**(42)
$2s^22p^4(^3_2P)3d\ ^4F$	7/2	779.7869	4.09×10^{-7}	**96** $2s^22p\text{-}^12p^3(1)3d$	**43**+**41**(20)
$2s^22p^4(^3_2P)3d\ ^4P$	5/2	780.8088	1.85×10^{-11}	**98** $2s^22p\text{-}^12p^3(1)3d$	**43**+**37**(49)
$2s^22p^4(^1_2D)3d\ ^2P$	3/2	780.8718	6.67×10^{-12}	**68** $2s^22p\text{-}^12p^3(1)3d$	**27** + **20**(42)+ **16**(50)
$2s^22p^4(^1_2D)3d\ ^2G$	9/2	781.289	3.82×10^{-9}	**100** $2s^22p\text{-}^12p^3(2)3d$	**67**+**32**(21)
$2s^22p^4(^1_2D)3d\ ^2D$	5/2	781.9558	2.64×10^{-11}	**98** $2s^22p\text{-}^12p^3(2)3d$	**52**
$2s^22p^4(^1_2D)3d\ ^2F$	7/2	782.4398	9.81×10^{-10}	**96** $2s^22p\text{-}^12p^3(2)3d$	**59**
$2s^22p^4(^3_2P)3d\ ^2D$	3/2	784.1285	5.98×10^{-14}	**67** $2s^22p\text{-}^12p^3(2)3d$	**42** + **23**(50)+ **23**(47)
$2s^22p^4(^1_2D)3d\ ^2P$	1/2	784.5867	3.55×10^{-14}	**97** $2s^22p\text{-}^12p^3(2)3d$	**34** + **32**(22)+ **31**(45)
$2s^22p^4(^3_2P)3s\ ^4P$	1/2	829.7138	8.87×10^{-11}	**99** $2s^22p^43s$	**43** + **34**(**??**)+ **22**(27)
$2s^22p^4(^3_2P)3p\ ^4D$	1/2	840.7876	2.28×10^{-12}	**99** $2s^22p^43p\text{-}^1$	**35** + **34**(**??**)+ **16**(36)
$2s^22p^4(^1S)3p\ ^2P$	3/2	868.6295	1.78×10^{-13}	**96** $2s^22p^43p^1$	**34** + **18**(35)+ **17**(31)
$2s^22p^4(^3_2P)3d\ ^4F$	3/2	880.3841	8.65×10^{-10}	**99** $2s^22p^43d\text{-}^1$	**34**
$2s^22p^4(^3_2P)3d\ ^2F$	5/2	886.2545	1.0×10^{-11}	**99** $2s^22p^43d^1$	**34** + **17**(60)+ **16**(16)

In our MCDF calculation, we predicted $1s^22s^22p^4(^3P_2)3p\ ^2D_{5/2}$ is strongly mixed with $1s^22s^22p^4(^1D_2)3p\ ^2D_{3/2}$ and $1s^22s^22p^4(^1D_2)3p\ ^2F_{5/2}$ with their compositions as 29%, 26% and 24%, respectively. Moreover, 26% of $2s^22p^4(^3P_2)3p\ ^2D_{5/2}$level mixed strongly with 21% of $2s^22p^4(^3P_2)3p\ ^4P_{5/2}$ and 20% of $2s^22p^4(^1D_2)3p\ ^2D_{5/2}$. Therefore, the identification of a particular level is difficult.

In Table 2, our calculated energy values of the fine-structure levels relative to ground level for F-like W from MCDF method are compared with the compiled values of NIST and also with the values calculated using FAC. We have also presented the experimental results of Beiersdorfer *et al.*[12] The NIST compiled energy values were originally measured by Clementson *et al.*[9] at superEBIT using the ECS X-ray calorimeter and the flat-crystal spectrometer. One can see from Table 2, our calculated value of energies from MCDF and FAC are in excellent agreement with the NIST values for the configuration $2s^22p^5$. Also, due to absence of NIST energy values for other configurations, we have compared our calculated values from NIST and FAC with those of Beiersdorfer *et al.*,[12] which are found to be in good agreement. It shows our results are reliable.

Table 2. MCDF Dirac–Coulomb (DC), Breit, and quantum electrodynamics (QED) contributions to the energy (in Ryd.) as a function of the orbital set.

Label	J	MCDF				FAC	NIST	Ref. [12]
		DC	Breit	QED	Total			
$2s^22p^5\ ^2P^o$	3/2	0						
$2s^22p^5\ ^2P^o$	1/2	103.2261	–1.3	0.12	102.0486	102.1934	102.08	
$2s2p^6\ \ ^2S$	1/2	138.8874	–0.0359	–1.16	137.694	137.4794	137.18	
$2s^22p^4(^3_2P)3s\ ^4P$	5/2	622.166	–1.27	0.169	621.0697	621.3361		621.7206
$2s^22p^4(^3_2P)3s\ ^2P$	3/2	622.9337	–1.22	0.169	621.8796	622.1517		622.5
$2s^22p^4(^1S)3s\ ^2S$	1/2	626.2932	–0.601	0.168	625.8603	626.2654		626.4485
$2s^22p^4(^3_2P)3p\ ^4P$	3/2	632.1864	–0.776	–0.17	631.2407	631.3898		631.8162
$2s^22p^4(^3_2P)3p\ ^2D$	5/2	632.5287	–0.974	–0.17	631.3844	631.5343		631.8162
$2s^22p^4(^1S)3p\ ^2P$	1/2	636.1966	–0.25	–0.171	635.7751	636.0552		
$2s^22p^4(^3_2P)3p\ ^4P$	5/2	661.3442	–1.33	–0.136	659.8754	660.0321		
$2s^22p^4(^3_2P)3p\ ^2S$	1/2	661.3675	–1.29	–0.136	659.9464	660.0564		
$2s^22p^4(^3_2P)3p\ ^4D$	7/2	661.379	–1.37	–0.135	659.8753	660.1467		
$2s^22p^4(^3_2P)3p\ ^4S$	3/2	664.6422	–0.987	–0.136	663.5196	663.7157		
$2s^22p^4(^3_2P)3p\ ^2P$	3/2	666.3022	–0.747	–0.136	665.4188	665.7291		
$2s^22p^4(^3_2P)3d\ ^4D$	3/2	671.9713	–1.08	–0.182	670.714	670.8766		
$2s^22p^4(^3_2P)3d\ ^4D$	5/2	672.4177	–1.35	–0.182	670.885	671.0093		
$2s^22p^4(^3_2P)3d\ ^4P$	1/2	672.5535	–1.21	–0.182	671.1567	671.0481		
$2s^22p^4(^3_2P)3d\ ^2F$	7/2	672.6172	–1.5	–0.182	670.9401	671.2852		
$2s^22p^4(^1S)3d\ ^2D$	3/2	676.2989	–0.709	–0.183	675.4067	675.6592		
$2s^22p^4(^3_2P)3d\ ^4D$	7/2	679.1231	–1.57	–0.182	677.3713	677.5026		
$2s^22p^4(^3_2P)3d\ ^4F$	9/2	679.2449	–1.65	–0.182	677.4175	677.5429		
$2s^22p^4(^3_2P)3d\ ^2P$	1/2	680.0958	–1.45	–0.182	678.4638	678.5916		
$2s^22p^4(^3_2P)3d\ ^2D$	5/2	681.9225	–1.48	–0.182	680.2594	680.3807		680.6103
$2s^22p^4(^3_2P)3d\ ^2P$	3/2	682.0101	–1.47	–0.182	680.3573	680.4813		680.6103
$2s^22p^4(^1S)3d\ ^2D$	5/2	684.1293	–0.982	–0.183	682.9646	683.2239		683.1985
$2s^22p^4(^3_2P)3s\ ^4P$	3/2	725.6316	–2.28	0.287	723.6366	724.0565		
$2s^22p^4(^3_2P)3s\ ^2P$	1/2	726.3546	–2.29	0.288	724.3534	724.7621		
$2s^22p^4(^1_2D)3s\ ^2D$	5/2	727.74	–2.9	0.288	725.1301	725.5271		
$2s^22p^4(^1_2D)3s\ ^2D$	3/2	728.1154	–2.81	0.287	725.5919	726.005		
$2s^22p^4(^3_2P)3p\ ^4P$	1/2	735.4063	–1.92	–0.0513	733.4395	733.7155		
$2s^22p^4(^3_2P)3p\ ^4D$	3/2	736.0901	–2.12	–0.0513	733.9161	734.1857		
$2s^22p^4(^1_2D)3p\ ^2F$	5/2	737.653	–2.65	–0.0516	734.9512	735.212		
$2s^22p^4(^1_2D)3p\ ^2P$	3/2	740.3578	–2.21	–0.0531	738.0933	738.4388		
$2s^22p^4(^3_2P)3p\ ^4D$	5/2	764.8886	–2.32	–0.0405	762.5287	762.5811		
$2s^22p^4(^3_2P)3p\ ^2D$	3/2	765.3555	–2.42	–0.0489	762.8885	763.0212		
$2s^22p^4(^3_2P)3p\ ^2P$	1/2	765.6673	–2.13	–0.17	763.3714	763.1744		
$2s^22p^4(^1_2D)3p\ ^2F$	7/2	766.7194	–3.03	–0.0163	763.6761	763.9588		
$2s^22p^4(^1_2D)3p\ ^2D$	3/2	767.2224	–2.49	–0.109	764.6281	764.3039		
$2s^22p^4(^1_2D)3p\ ^2D$	5/2	767.4896	–2.83	–0.0233	764.6376	764.8426		
$2s^22p^4(^1_2D)3p\ ^2P$	1/2	771.2687	–2.47	–0.0405	768.7536	768.8952		
$2s^22p^4(^3_2P)3d\ ^4D$	1/2	775.0341	–2.24	–0.063	772.7272	772.9871		
$2s^22p^4(^3_2P)3d\ ^4P$	3/2	776.0811	–2.42	–0.0673	773.5953	773.8268		
$2s^22p^4(^3_2P)3d\ ^4F$	5/2	776.6283	–2.54	–0.066	774.0254	774.2211		
$2s^22p^4(^1_2D)3d\ ^2G$	7/2	777.7324	–3.13	–0.0625	774.5434	774.7681		

Table 2. (*continued*)

Label	J	MCDF				FAC	NIST	Ref. [12]
		DC	Breit	QED	Total			
$2s^22p^4(^1_2D)3d\ ^2S$	1/2	779.0022	–2.75	–0.0961	776.1573	776.1387		776.6324
$2s^22p^4(^1_2D)3d\ ^2F$	5/2	779.253	–2.97	–0.0693	776.2118	776.3479		776.6324
$2s^22p^4(^1_2D)3d\ ^2D$	3/2	779.5313	–2.83	–0.0834	776.6228	776.6711		776.6324
$2s^22p^4(^3_2P)3d\ ^4F$	7/2	782.5013	–2.65	–0.0674	779.7869	780.0826		
$2s^22p^4(^3_2P)3d\ ^4P$	5/2	783.4051	–2.53	–0.0636	780.8088	781.0477		
$2s^22p^4(^1_2D)3d\ ^2P$	3/2	783.622	–2.68	–0.0653	780.8718	781.1465		
$2s^22p^4(^1_2D)3d\ ^2G$	9/2	784.6103	–3.26	–0.0624	781.289	781.5198		
$2s^22p^4(^1_2D)3d\ ^2D$	5/2	785.063	–3.04	–0.067	781.9558	782.2307		
$2s^22p^4(^1_2D)3d\ ^2F$	7/2	785.5822	–3.08	–0.0644	782.4398	782.6704		
$2s^22p^4(^3_2P)3d\ ^2D$	3/2	787.1796	–2.99	–0.0648	784.1285	784.3758		
$2s^22p^4(^1_2D)3d\ ^2P$	1/2	787.7914	–3.14	–0.0658	784.5867	784.856		
$2s^22p^4(^3_2P)3s\ ^4P$	1/2	832.8129	–3.49	0.394	829.7138	830.6073		
$2s^22p^4(^3_2P)3p\ ^4D$	1/2	843.9272	–3.19	0.0535	840.7876	841.5901		
$2s^22p^4(^1S)3p\ ^2P$	3/2	872.0656	–3.5	0.0614	868.6295	869.1568		
$2s^22p^4(^3_2P)3d\ ^4F$	3/2	884.0567	–3.71	0.0357	880.3841	881.0046		
$2s^22p^4(^3_2P)3d\ ^2F$	5/2	889.9588	–3.75	0.0415	886.2545	886.9918		

3.2. Radiative rates

We have reported the transition wavelengths (λ in Å), transition probabilities (A_{ji} in s^{-1}), oscillator strengths (f_{ij}, dimensionless) and line strengths (S in a.u) for electric dipole (E1) transitions from $^2P_{3/2}$ and $^2P_{1/2}$ levels in Tables 3 and 4 respectively. We have presented results only in length form. To assess the quality and reliability of our MCDF wavefunctions, we have also compared our calculated values of transition probability using MCDF with the calculated values of FAC. From Tables 3 and 4, one can see that the values of transition probabilities calculated using the MCDF and FAC are in close agreement with each other.

Table 3. Transition data for E1 transitions from $2s^22p^5\ ^2P_{3/2}$: levels and $2J$ for lower level I, upper level k, wavelength λ (in Å), line strength S (length form), oscillator strength f (length form), and transition rate A_{ji} (length form).

Levels		2J		λ/Å	A_{ji}/s^{-1} (MCDF)	A_{ji}/s^{-1} (FAC)	f_{ij}	S_{ij}/au	vel/len
i	k	I	K						
$2s^22p^5\ ^2P^o$	$-2s2p^6\ ^2S$	3	1	6.62	2.22×10^{13}	2.04×10^{13}	7.28×10^{-2}	6.35×10^{-3}	0.99
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3s\ ^4P$	3	5	1.47	3.83×10^{13}	3.65×10^{13}	1.86×10^{-2}	3.59×10^{-4}	0.99
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3s\ ^2P$	3	3	1.47	2.30×10^{14}	2.22×10^{14}	7.41×10^{-2}	1.43×10^{-3}	0.99
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^1S)3s\ ^2S$	3	1	1.46	1.14×10^{14}	1.09×10^{14}	1.82×10^{-2}	3.48×10^{-4}	1
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^4D$	3	3	1.36	2.29×10^{13}	2.11×10^{13}	6.35×10^{-3}	1.14×10^{-4}	0.98
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^4D$	3	5	1.36	7.40×10^{13}	6.90×10^{13}	3.07×10^{-2}	5.49×10^{-4}	0.99
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^4P$	3	1	1.36	3.48×10^{14}	3.31×10^{14}	4.81×10^{-2}	8.60×10^{-4}	0.98
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^1S)3d\ ^2D$	3	3	1.35	5.16×10^{12}	3.73×10^{12}	1.41×10^{-3}	2.50×10^{-5}	1
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^2P$	3	1	1.34	7.86×10^{14}	7.97×10^{14}	1.06×10^{-1}	1.88×10^{-3}	0.98
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^2D$	3	5	1.34	1.62×10^{15}	1.67×10^{15}	6.55×10^{-1}	1.16×10^{-2}	0.99
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^2P$	3	3	1.34	2.00×10^{15}	2.02×10^{15}	5.37×10^{-1}	9.48×10^{-3}	0.98
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^1S)3d\ ^2D$	3	5	1.33	1.09×10^{15}	1.10×10^{15}	4.37×10^{-1}	7.68×10^{-3}	0.99
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3s\ ^4P$	3	3	1.26	2.01×10^{13}	2.13×10^{13}	4.78×10^{-3}	7.93×10^{-5}	0.99
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3s\ ^2P$	3	1	1.26	5.11×10^{13}	5.19×10^{13}	6.06×10^{-3}	1.00×10^{-4}	0.99
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^1_2D)3s\ ^2D$	3	5	1.26	4.14×10^{13}	4.20×10^{13}	1.47×10^{-2}	2.43×10^{-4}	0.98
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^1_2D)3s\ ^2D$	3	3	1.26	1.98×10^{13}	2.03×10^{13}	4.68×10^{-3}	7.74×10^{-5}	0.99
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^4D$	3	1	1.18	1.64×10^{12}	3.44×10^{11}	1.71×10^{-4}	2.66×10^{-6}	0.96
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^4P$	3	3	1.18	3.51×10^{12}	2.35×10^{12}	7.30×10^{-4}	1.13×10^{-5}	0.96
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^4F$	3	5	1.18	3.34×10^{14}	4.22×10^{14}	1.04×10^{-1}	1.61×10^{-3}	0.99
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^1_2D)3d\ ^2S$	3	1	1.17	1.28×10^{15}	1.79×10^{15}	1.33×10^{-1}	2.05×10^{-3}	0.97
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^1_2D)3d\ ^2F$	3	5	1.17	1.29×10^{15}	1.41×10^{15}	3.99×10^{-1}	6.17×10^{-3}	0.99
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^1_2D)3d\ ^2D$	3	3	1.17	1.45×10^{15}	1.79×10^{15}	3.00×10^{-1}	4.63×10^{-3}	0.98
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^4P$	3	5	1.17	5.41×10^{10}	7.11×10^{10}	1.66×10^{-5}	2.55×10^{-7}	0.92
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^1_2D)3d\ ^2P$	3	3	1.17	1.50×10^{11}	5.61×10^{11}	3.06×10^{-5}	4.70×10^{-7}	1
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^1_2D)3d\ ^2D$	3	5	1.17	3.79×10^{10}	2.46×10^{10}	1.16×10^{-5}	1.78×10^{-7}	0.69
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^2D$	3	3	1.16	1.67×10^{13}	1.68×10^{13}	3.39×10^{-3}	5.19×10^{-5}	1
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^1_2D)3d\ ^2P$	3	1	1.16	2.81×10^{13}	3.02×10^{13}	2.85×10^{-3}	4.35×10^{-5}	0.98
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3s\ ^4P$	3	1	1.10	1.13×10^{10}	1.00×10^{10}	1.02×10^{-6}	1.47×10^{-8}	1.1
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^4F$	3	3	1.04	1.16×10^{9}	1.32×10^{9}	1.86×10^{-7}	2.53×10^{-9}	0.5
$2s^22p^5\ ^2P^o$	$-2s^22p^4(^3_2P)3d\ ^2F$	3	5	1.03	9.95×10^{10}	1.00×10^{11}	2.37×10^{-5}	3.20×10^{-7}	1.1

Table 4. Transition data for E1 transitions from $2s^2 2p^5\ ^2P_{1/2}$: levels and $2J$ for lower level I, upper level k, wavelength λ (in Å), line strength S (length form), oscillator strength f (length form), transition rate A_{ji} (length form). The last column represents the ratio of vel. and len. form of oscillator strength.

Levels		$2J$		λ/Å	A_{ji}/s^{-1}	A_{ji}/s^{-1}	f_{ij}	S_{ij}/au	vel/len
i	k	I	K		(MCDF)	(FAC)			
$2s^2 2p^5\ ^2P^o$	$-2s2p^6\ ^2S$	1	1	2.56×10^{1}	1.65×10^{11}	1.54×10^{11}	1.62×10^{-2}	2.73×10^{-3}	0.91
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3s\ ^2P$	1	3	1.75	3.40×10^{9}	2.47×10^{9}	3.14×10^{-6}	3.62×10^{-8}	1.4
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^1S)3s\ ^2S$	1	1	1.74	1.86×10^{10}	2.99×10^{10}	8.44×10^{-6}	9.67×10^{-8}	0.51
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3d\ ^4D$	1	3	1.60	7.64×10^{10}	8.65×10^{10}	5.88×10^{-5}	6.21×10^{-7}	0.75
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3d\ ^4P$	1	1	1.60	5.60×10^{10}	5.12×10^{10}	2.15×10^{-5}	2.27×10^{-7}	1.1
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^1S)3d\ ^2D$	1	3	1.59	4.93×10^{10}	5.01×10^{10}	3.74×10^{-5}	3.91×10^{-7}	0.82
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3d\ ^2P$	1	1	1.58	9.05×10^{7}	7.06×10^{7}	3.39×10^{-8}	3.53×10^{-10}	1.5
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3d\ ^2P$	1	3	1.58	9.02×10^{9}	8.56×10^{9}	6.71×10^{-6}	6.97×10^{-8}	1.8
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3s\ ^4P$	1	3	1.47	1.83×10^{12}	1.96×10^{12}	1.18×10^{-3}	1.14×10^{-5}	1
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3s\ ^2P$	1	1	1.46	1.57×10^{14}	1.50×10^{14}	5.04×10^{-2}	4.86×10^{-4}	1
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^1_2D)3s\ ^2D$	1	3	1.46	1.56×10^{14}	1.48×10^{14}	1.00×10^{-1}	9.62×10^{-4}	0.99
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3d\ ^4D$	1	1	1.36	4.07×10^{13}	3.84×10^{13}	1.13×10^{-2}	1.01×10^{-4}	0.98
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3d\ ^4P$	1	3	1.36	5.94×10^{13}	5.48×10^{13}	3.28×10^{-2}	2.93×10^{-4}	0.99
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^1_2D)3d\ ^2S$	1	1	1.35	3.64×10^{13}	3.54×10^{13}	9.97×10^{-3}	8.87×10^{-5}	0.96
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^1_2D)3d\ ^2D$	1	3	1.35	1.73×10^{13}	1.74×10^{13}	9.45×10^{-3}	8.41×10^{-5}	1
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^1_2D)3d\ ^2P$	1	3	1.34	1.04×10^{14}	1.12×10^{14}	5.63×10^{-2}	4.98×10^{-4}	0.99
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3d\ ^2D$	1	3	1.34	2.83×10^{15}	2.88×10^{15}	1.52	1.33×10^{-2}	0.99
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^1_2D)3d\ ^2P$	1	1	1.34	3.05×10^{15}	3.08×10^{15}	8.14×10^{-1}	7.15×10^{-3}	0.98
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3s\ ^4P$	1	1	1.25	5.07×10^{13}	5.25×10^{13}	1.19×10^{-2}	9.83×10^{-5}	1
$2s^2 2p^5\ ^2P^o$	$-2s^2 2p^4(^3_2P)3d\ ^4F$	1	3	1.17	1.23×10^{15}	1.39×10^{15}	5.05×10^{-1}	3.89×10^{-3}	0.99

In general, we can check the reliability of our calculated A and f values by comparing the length and velocity forms in the MCDF method. One can see from Tables 3 and 4, the difference between both forms for strong E1type transitions ($f \geq 0.1$) ($^2P_{3/2}$ and $^2P_{1/2}$ levels to even levels) does not exceed 2%. However, for a majority of weak transitions, the difference between two forms of transitions ($f < 0.1$) can sometimes be large, particularly for those with f values below 10^{-4}. This is due to mixing present in these levels with other levels. Therefore, all such weak transitions do not affect the overall accuracy of the calculations.

4. Conclusions

In present work, we have reported the energies, wave function compositions and lifetimes of $1s^2 2s^2 2p^5$, $1s^2 2s 2p^6$ $1s^2 2s^2 2p^4 3s$, $1s^2 2s^2 2p^4 3p$, and $1s^2 2s^2 2p^4 3d$ configurations. We have performed the accuracy test by comparing our calculated results using MCDF and FAC with the other available experimental measurements and theoretical calculations. The components of the wave function has been calculated in both *JJ* and *LSJ* coupling. Our calculated results are in good agreement with the experimental measurements and with the calculations performed previously. Based on the comparison made with the available experimental and other theoretical results, our energy levels are found to be accurate (better than 3%) for majority of levels. We can conclude that the achieved accuracy of our calculations is higher than those available to date.

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References

[1] Zigler A, Zmora H, Spector N, Klapisch M, Schwob J L and Bar-Shalom A 1980 *J. Opt. Soc. Am.* **70** 129
[2] Mandelbaum P, Klapisch M, Bar-Shalom A, Schwob J L and Zigler A 1983 *Phys. Scr.* **27** 39
[3] Tragin N, Geindre J P, Monier P, Gauthier J C, Chenaispopovics C, Wyart J F and Bauche-Arnoult C 1988 *Phys. Scr.* **37** 72
[4] Neu R, Fournier K B, Schögl D and Rice J 1997 *J. Phys. At. Mol. Opt. Phys.* **30** 5057
[5] Pütterich T, Neu R, Biedermann C, Radtke R and the ASDEX upgrade team 2005 *J. Phys. At. Mol. Opt. Phys.* **38** 307
[6] Aggarwal S, Jha A K S and Mohan M 2013 *Can. J. Phys.* **91** 394
[7] Mohan M, Aggarwal S and Singh N 2014 *Can. J. Phys.* **92** 1
[8] Podpaly Y, Clementson J, Beiersdorfer P, Williamson J, Brown G V and Gu M F 2009 *Phys. Rev. A* **80** 052504
[9] Clementson J, Beiersdorfer P, Brown G V, Gu M F, Lundberg H, Podpaly Y and Trabert E 2011 *Can. J. Phys.* **89** 571
[10] Feldman U, Seely J F, Landi E and Ralchenko Y 2008 *Nucl. Fusion* **48** 045004
[11] Pütterich T, Neu R, Dux R, Whiteford A D, Mullane M G O and the ASDEX upgrade team 2008 *Plasma Phys. Control Fusion* **50** 085016
[12] Beiersdorfer P, Lepson J K, Schneider M B and Bode M P 2012 *Phys. Rev. A* **86** 012509
[13] Kramida A E and Reader J 2006 *At. Data Nucl. Data Tables* **92** 457
[14] Kramida A E and Shirai T 2009 *At. Data Nucl. Data Tables* **95** 305
[15] Kramida A E 2011 *Can. J. Phys.* **89** 551
[16] http://www.nist.gov/pml/data/asd.cfm
[17] Grant I P, Mckenzie B J, Norrington P H, Mayers D F and Pyper N C 1980 *Comput. Phys. Commun.* **21** 207
[18] Dyall K G, Grant I P, Johnson C T and Plummer E P 1989 *Comput. Phys. Commun.* **55** 425
[19] Parpia F A, Fischer C F and Grant I P 1996 *Comput. Phys. Commun.* **94** 249
[20] J'onsson P, He X, Fischer C F and Grant I P 2007 *Comput. Phys. Commun.* **177** 597
[21] Norrington P H 2009 http://www.am.qub.ac.uk/DARC/
[22] Quinet P 2012 *J. Phys. B* **45** 025003
[23] Aggarwal S, Singh J and Mohan M 2013 *Chin. Phys. B* **22** 033201
[24] Singh A K, Aggarwal S and Mohan M 2013 *Phys. Scr.* **88** 035301
[25] Aggarwal S, Singh J and Mohan M 2013 *At. Data Nucl. Data Tables* **99** 704
[26] Gu M F 2008 *Can. J. Phys.* **86** 675