# Benchmarking calculations with spectroscopic accuracy of excitation energies and wavelengths in sulfur-like tungsten

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Atomic properties of S-like W are evaluated through a state-of-the-art method, namely, the multiconfiguration Dirac-Hartree-Fock (MCDHF) method combined with the relativistic configuration interaction (RCI) approach. The level energies, wavelengths, and transition parameters involving the 88 lowest levels of  $W^{+58}$  (W LIX) are calculated. We discuss in detail the relative importance of the valence- and core-valence electron correlation effects, the Breit interaction, the higher order retardation correction beyond the Breit interaction through the transverse photon interaction, and the quantum electrodynamical (QED) corrections. The present level energies are highly accurate, with uncertainties close to what can be achieved from spectroscopy. As such, they provide benchmark tests for other theoretical calculations of S-like W and should assist the spectroscopists in their assignment/identification of observed lines in complex spectra.

## I. INTRODUCTION

The *M*-shell (n = 3) tungsten ions, such as S-like W<sup>+58</sup>, are of great importance due to their potential use in plasma diagnostics in the future tokamak fusion reactor ITER [1–7]. Of special interest are the many strong emission lines in the 10 – 60 Å, region, which are needed to monitor the tungsten-ion impurity levels and to properly predict the radiative emissions.

These applications stimulated some calculations of excitation energies and wavelengths for S-like W [8–11]. However, a satisfactory accuracy has not been achieved yet. For example, the two data sets reported by Aggarwal et al. [8], using the general-purpose relativistic atomic structure package (GRASP89) [12] and the flexible atomic code (FAC) [13], are inconsistent, with excitation energy deviations of up to 30 000 cm<sup>-1</sup>. The excitation energies calculated by Xu et al. [9] differ by 3 000 - 70 000 cm<sup>-1</sup> from the results of Ref. [8], although both sets are evaluated using the same GRASP89 code [12]. Unfortunately, these inconsistencies cannot be resolved by experimental measurements because the theory-observation energy deviations for both sets are much larger than the experimental error bars.

On the other hand, the identification of measured lines also needs the support of theoretical calculations, but the latter do not provide the needed accuracy. Lennartsson et al. [2] measured several lines of the *M*-shell tungsten ions using the electron beam ion trap (EBIT) facility of the Lawrence Livermore National Laboratory (LLNL). Two lines at  $\lambda = 34.779(4)$  Å and 35.644(4) Å have not been identified, due to the lack of robust and reliable calculations. The FAC relativistic configuration interaction (RCI) calculations reported in [2] were indeed not accurate enough. To illustrate this, the line observed at 34.779(4) Å might correspond to one of the following three transitions:  $3s^2 3p^{4-1}D_2 \rightarrow 3s^2 3p^{4-3}P_2$  (an M1 transition of S-like W),  $3s^2 3p^3 ({}^2P) 3d {}^1P_1^o \rightarrow 3s^2 3p^4 {}^3P_2$  (an E1 transition of S-like W), and  $3s^2 3p^5 (^2P) 3d^2 {}^4D^o_{5/2} \rightarrow$  $3s^2 3p^6 3d \ ^2D_{3/2}$  (an E1 transition of K-like W), with calculated wavelengths, Lennartsson et al. [2], of 34.735 Å, 34.800 Å, and 34.812 Å, respectively. All three wavelengths are "equally close" to the measured one, but all

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lying outside the experimental error bars of 0.004 Å.

The line at 35.644(4) Å measured by Lennartsson et al. [2] was not identified for the same reason. Furthermore, many atomic energy levels of S-like W compiled in the Atomic Spectra Database (ASD) of the National Institute of Standards and Technology (NIST) [14], which are determined by interpolation or extrapolation of known experimental values or by semiempirical calculation, have relatively large energy uncertainties, from 20 000 cm<sup>-1</sup> to 60 000 cm<sup>-1</sup>, due to the lack of accurate theoretical reference values.

In this paper, using the multi-configuration Dirac-Hatree-Fock (MCDHF) method and the relativistic configuration interaction approach (RCI) [15] as implemented in the GRASP2K code [16, 17], we improve on the accuracy of previous theoretical results. The deviations between our wavelengths and experiments are within 0.06 %. The various contributions to the excitation energies, such as valence-valence (VV) and core-valence (CV) electron correlation, along with the Breit and transverse photon interactions, are investigated in detail. We also conduct a detailed study of the quantum electrodynamic (QED) corrections, comparing the performance of three different methods for describing the self energy. This effort paves the way for future applications of this approach for accurate predictions of properties of multielectron high-Z ions and provides precision benchmarks for spectral identifications and other applications.

# II. THEORETICAL METHOD AND COMPUTATIONAL MODELS

#### A. Electron correlation with the MCDHF method

In the MCDHF method [16], electron correlation is included by expanding the atomic state function (ASF)  $\Psi(\Gamma PJ)$  in configuration state functions (CSFs)

$$\Psi\left(\Gamma PJ\right) = \sum_{i=1}^{M} c_i \Phi\left(\gamma_i PJ\right). \tag{1}$$

The CSFs,  $\Phi(\gamma_i PJ)$ , are *jj*-coupled many-electron functions built from antisymmetrized products of oneelectron Dirac orbitals, where  $\gamma_i$  specifies the occupied subshells with their complete angular coupling tree information, P the parity and J the total angular momentum. The radial large and small components of the one-electron orbitals and the expansion coefficients  $\{c_i\}$  of the CSFs are obtained by solving iteratively the Dirac-Hartree-Fock radial equations and the configuration interaction eigenvalue problem resulting from applying the variational principle on the energy functional of the targeted states in the extended optimal level (EOL) scheme [16, 18]. The energy functional is based on the Dirac-Coulomb (DC) Hamiltonian

$$\mathcal{H}_{DC} = \sum_{i=1}^{N} \left( c \, \boldsymbol{\alpha}_i \cdot \mathbf{p}_i + V_{nuc}(r_i) + c^2(\beta_i - 1) \right) + \sum_{j>i=1}^{N} \frac{1}{r_{ij}}, \tag{2}$$

and accounts for relativistic kinematic effects.

The configurations  $\{3s^23p^4, 3s^23p^23d^2, 3s3p^43d,$  $3s3p^23d^3$ ,  $3p^6$ ,  $3p^43d^2$  { $3s^23p^33d$ ,  $3s^23p3d^3$ ,  $3s3p^5$ ,  $3s3p^33d^2$ ,  $3p^53d$  constitute, respectively, the multireference (MR) spaces for even and odd parities. The CSF expansions are generated by allowing single (S) and double (D) excitations of all the n = 3 electrons, namely valence electrons, from all MR configurations to  $n \leq 7, l \leq 5$ (i.e., up to *h*-orbital symmetry). These CSFs describe the valence-valence (VV) electron correlation. No substitutions were allowed from the 1s shell, which defines an inactive closed core. In a second series of calculations we added, to the CSFs above, CSFs resulting from excitations of the n = 2 electrons to orbitals with  $n \leq 6, l \leq 5$ . These added CSFs describe the core-valence (CV) correlation effects. The core-core electron correlation effects are unimportant for the excitation energies of the studied states and have thus been neglected, compare [19]. The numbers of CSFs distributed over the different J symmetries in the final even and odd state expansions are, respectively, 20 396 713 and 11 691 659.

#### B. Breit and QED Corrections

In the relativistic description of the many-electron system, the Dirac-Coulomb Hamiltonian (2) is the starting point that should be corrected by the so called transverse photon (TP) interaction, which, in the  $\alpha^2$  approximation, takes the form:

$$H_{\rm TP} = -\sum_{i$$

where  $\omega_{ij}$  is the frequency of the exchanged virtual photon propagating the interaction [20]. In the lowfrequency limit  $\omega_{ij} \to 0$ , the TP interaction reduces to the Breit interaction [21]

$$\mathcal{H}_{\text{Breit}} = -\sum_{j>i=1}^{N} \frac{1}{2r_{ij}} \left[ (\boldsymbol{\alpha}_{i} \cdot \boldsymbol{\alpha}_{j}) + \frac{(\boldsymbol{\alpha}_{i} \cdot \mathbf{r}_{ij})(\boldsymbol{\alpha}_{j} \cdot \mathbf{r}_{ij})}{r_{ij}^{2}} \right].$$
(4)

which is the sum of the Gaunt interaction

$$\mathcal{H}_{\text{Gaunt}} = -\sum_{j>i=1}^{N} \frac{\boldsymbol{\alpha}_{i} \cdot \boldsymbol{\alpha}_{j}}{r_{ij}}$$
(5)

and the Breit retardation [22]

$$\mathcal{H}_{\text{Breit}}^{\text{retard.}} = +\sum_{j>i=1}^{N} \frac{1}{2r_{ij}} \left[ (\boldsymbol{\alpha}_{i} \cdot \boldsymbol{\alpha}_{j}) - \frac{(\boldsymbol{\alpha}_{i} \cdot \mathbf{r}_{ij})(\boldsymbol{\alpha}_{j} \cdot \mathbf{r}_{ij})}{r_{ij}^{2}} \right]$$
(6)

The higher-order retardation correction beyond the Breit interaction (4) is therefore defined as the difference

$$\mathcal{H}^{\rm HO} \equiv \mathcal{H}_{\rm TP} - \mathcal{H}_{\rm Breit} = \mathcal{H}_{\rm TP} - \left(\mathcal{H}_{\rm Gaunt} + \mathcal{H}_{\rm Breit}^{\rm retard.}\right) \ . \ (7)$$

Once the orbitals optimized through the MCDHF procedure are available, the transverse photon interaction, or the Breit interaction, and the leading QED effects (vacuum polarization and self-energy) can be added to the Dirac-Coulomb Hamiltonian in relativistic configuration interaction (RCI) calculations to capture relativistic corrections to the Coulomb interaction.

For evaluating the TP Hamiltonian matrix elements, some decision has to be taken for the appropriate value of the  $\omega_{ij}$ . These matrix elements involve indeed two-body contributions of the form  $(a_q^{\dagger}a_p)(a_s^{\dagger}a_r)$  with their own single-electron energies  $\{\epsilon_p, \epsilon_q, \epsilon_r, \epsilon_s\}$  for which  $\omega_{ij}$  can be taken as  $\omega_{ij} = \omega_{sr} = -\omega_{qp}$  when the effective potentials are derived "on the energy shell" [16]. Averaging  $\omega_{sr}$  and  $\omega_{pq}$  has proved quite effective in bound state calculations involving atomic inner shells for "off-shell" potentials but the individual one-particle energies  $\epsilon_i$  are physically meaningful only for spectroscopic orbitals. In the present work, the frequency-dependent contributions to the TP Hamiltonian matrix elements are included only between CSFs built from the spectroscopic orbitals. For matrix elements between CSFs involving correlation orbitals, the low-frequency limit is considered.

The current status of bound state quantum electrodynamics calculations of transition energies for a fewelectron highly-charged ions has been reviewed very recently by Indelicato [23]. The one-electron QED corrections are separated into two contributions, namely, the self-energy (SE) and the vacuum polarization (VP). The VP contribution can be represented by a potential. We use for the present work the analytical expressions derived by Fullerton and Rinker [24] for the Uehling model potential and the higher-order Källén-Sabry VP potential. For S-like W, the self-energy contribution dominates the QED corrections. We investigate three different methods (M1 - M3) for estimating the latter:

• QED - M1: In the current GRASP2K code, starting from the self energy of a hydrogenic system

$$\Delta E_{SE} = \left(\frac{\alpha}{\pi}\right) \frac{\alpha^2 Z^4}{n^3} F(nlj, Z\alpha), \tag{8}$$

where  $F(nlj, Z\alpha)$  is a slowly varying function of  $Z\alpha$  that has been tabulated by Mohr et al. [25] and Klarsfeld et al. [26], the total SE contribution is given as a sum of one-electron corrections weighted by the fractional occupation number of the one-electron orbital in the total wave function. For each orbital, the effective nuclear charge or, equivalently the screening, is estimated by equating the mean radius of each MCDHF orbital to that of a hydrogenic (Dirac) orbital [16].

- QED M2: Starting from the latest available hydrogenic values [27, 28] modified to account for finite-nuclear-size effects [29, 30], a screening approximation based on the Welton interpretation [31] and implemented in GRASP2K by Lowe et al. [32], is used to evaluate the SE contribution.
- QED M3: A model QED operator, which also includes the non-local QED part to calculate the SE corrections for many-electron atomic systems, was recently developed by Shabaev et al. (QED-MOD) [33, 34]. We also include this model SE operator in the GRASP2K code to evaluate the SE contribution.

The last two approaches (QED - M2/M3) have recently been used for investigating Breit and QED effects in the ground-term fine structures of F-like [35] and Co-like [36] ions.

The following notations will be used for the various correlation and interaction models:

- 1. Multireference MCDHF calculations will be denoted VV when limiting the inclusion of electron correlation to the valence shells, and CV when enlarging the multiconfiguration expansions to core-valence excitations.
- 2. Taking the long wavelength limit for the transverse part and adding the resulting Breit interaction (4) to the Dirac-Coulomb Hamiltonian (2) defines the Dirac-Coulomb-Breit (DCB) Hamiltonian, in the effective Coulomb gauge

$$\mathcal{H}_{DCB} = \mathcal{H}_{DC} + \mathcal{H}_{Breit} . \tag{9}$$

3. Adding the transverse photon interaction in Coulomb gauge (3) to the Dirac-Coulomb Hamiltonian (2) gives the more complete Hamiltonian

$$\mathcal{H}_{DCTP} = \mathcal{H}_{DC} + \mathcal{H}_{TP} \tag{10}$$

4. Calculations including QED corrections estimated by selecting one of the three models (M1, M2 or M3) as described above, and added to  $\mathcal{H}_{DCTP}$  in the very last step, are denoted QED(Mx).

The relativistic corrections to the Coulomb interaction and quantum electrodynamics corrections considered in steps (2-4) are included in RCI calculation based on CS-F expansions accounting for both VV and CV electron correlation.

#### III. RESULTS

#### A. Excitation energies

#### 1. Electron correlation

In Table I, we present the excitation energies for a selection of levels from the above correlation and interaction models, together with the values compiled in

the NIST Atomic Spectra Database (ASD) [14], except for the values determined by semi-empirical calculation since they have relatively large energy uncertainties. Only the NIST values deduced from measured lines are compared with the present results in Table I. The atomic units are used throughout the present work, if units are not indicated explicitly. In Table I, the key is a number assigned to each level. The deviations  $(\Delta E = E_{\text{MCDHF/RCI}} - E_{\text{NIST}})$  between our calculated MCDHF/RCI excitation energies and the experimental values compiled in the NIST ASD are also reported. On average, CV electron correlation plays a smaller role than VV electron correlation, as expected for transitions involving valence excitations. CV electron correlation was systematically omitted in all previous theoretical calculations performed for S-like W [8, 9, 11, 24]. However, limiting electron correlation to VV electron correlation is not enough to reach the needed accuracy for assisting spectroscopists in the spectral lines identification process, as discussed in Ref. [2]. By comparing the two columns  $\Delta E$ -VV and  $\Delta E$ -CV of Table I, it is seen that the addition of CV to the VV electron correlation further reduces the energy differences between the MCDHF and observed (NIST) excitation energy values by  $\simeq 1 \ 100 - 5 \ 600 \ \mathrm{cm}^{-1}$ for the levels considered. This illustrates the importance of core-valence correlation, even for such highly charged ions.

## 2. The Breit interaction and QED corrections

As revealed by column 5 of Table I, the magnitude of the Breit correction to excitation energies strongly depends on the electronic configuration. The Breit correction affects the excitation energies of the levels of the  $3s^23p^33d$  configuration by  $\simeq 10\ 000 - 45\ 000\ \mathrm{cm}^{-1}$ . The corresponding effect on the levels arising from the  $3s3p^5$ configuration is considerably smaller, around  $5\ 000\ \mathrm{cm}^{-1}$ .

Comparing column 6 with column 5 of Table I, one observes that the higher-order frequency-dependent corrections  $\mathcal{H}^{\text{HO}} = \mathcal{H}_{\text{TP}} - \mathcal{H}_{\text{Breit}}$  are relatively small compared with the Breit interaction, but cannot be neglected for precision calculations of excitation energies in S-like W.

Adding the QED corrections to the MCDHF/RCI excitation energies improves substantially the agreement with observation. These QED corrections reach around 4 000 - 29 000 cm<sup>-1</sup>. The QED corrections to excitation energies are naturally grouped according to the electronic configuration of the level considered, as observed for the Breit interaction. As expected the QED contribution to the excitation energies of the levels of the  $3s3p^5$  configuration is significantly larger than the contribution to the excitation energies of the levels of the  $3s^23p^33d$  configuration due to the change in the 3s electron occupation number for the former configuration.

The QED corrections to the excitation energies obtained using the three different QED potentials as described above, are also given in Table I. Compared with the results obtained by using the QED-M1 method, the MCDHF/RCI results based on the QED - M2 and QED - M3 methods are closer to the experimental NIST values. The QED corrections obtained by using the QED - M2 and QED - M3 methods are very similar. For each level considered, the excitation energies obtained with both QED-M2/M3 models lie within the error bars of the estimated experimental uncertainty reported in the  $E_{\rm NIST}$  column.

In short, the Breit interaction and QED corrections play the most important role in the calculations of excitation energies of S-like W<sup>58+</sup>. However, the CV electron correlation and the higher-order corrections (7) arising from  $\mathcal{H}_{TP} - \mathcal{H}_{Breit}$ , which were not considered in the previous calculations [8–11], cannot be omitted for highprecision results. Since our MCDHF/RCI excitation energies obtained by using the QED - M2 and QED - M3 methods are very similar, the results that are reported in the following sections are only based on the M2 model. Moreover, the MCDHF/RCI label will be shortened from here by the single MCDHF generic denomination to simplify the notations, but the reader should be aware that Breit, TP and QED corrections were all included in the final RCI calculations.

#### B. Wavelengths and transition rates

In Table II we present the differences  $\Delta\lambda$  between the present theoretical wavelengths calculated at different levels of approximation and the experimental values. The differences between the present theoretical wavelengths and the measured values for the E1 transitions are found to be around several hundreds mÅ when VV and CV electron correlation is included in the DiracCoulomb approximation. Once the  $\mathcal{H}_{DCTP}$  Hamiltonian (10) is considered to take the transverse photon interaction into account, our wavelengths are getting closer to the measured ones, reducing the differences to  $-200 \leq \Delta \lambda \leq +24$  mÅ. By further adding the QED corrections, the wavelength differences become of the same order of magnitude than the estimated uncertainty of the experimental value reported in parentheses in the  $\lambda_{exp.}$ column. Since the upper and lower levels of the M1 transition  $3s^23p^{4-1}D_2 - 3s^23p^{4-3}P_2$  belong to the same configuration, the Breit/TP interaction and QED corrections have similar effects on the levels involved, affecting only slightly the wavelength of this intra-configuration transition.

As far as transition rates are concerned, the magnetic Breit/TP interaction decreases transition rates by  $\simeq 3$  %, on average. However, the variations in transition rates due to QED are about  $\simeq 0.3$  %. One observes that the QED corrections barely change the M1 transition rate. This characteristics was also found for the M1 transitions within the 3d<sup>n</sup> configurations (with n = 2-5) in Ref. [37].

# C. Comparison with other theoretical works and observation

Excitation energies of S-like W from the present MCD-HF/RCI calculations, as well as the compiled data from the NIST ASD [14], are listed in Table III. For comparison, the two theoretical data sets reported by Aggarwal et al. [8], and the theoretical results provided by Xu et al. [9] are also included in the table.

The NIST compiled values in square brackets are determined from semi-empirical calculations by Kramida [38] using Cowan's code [39]. The other NIST values are deduced from measured lines that were observed using the EBIT facilities [1, 40]. For each level, the number reported in parenthesis, after the NIST excitation level energy, is the estimated accuracy provided by the NIST ASD. It can be seen from this table that the accuracy of the NIST values quoted in square brackets is generally about tens of thousands cm<sup>-1</sup>, whereas the NIST values deduced by measured lines are much more accurate  $(110 - 2500 \text{ cm}^{-1}).$ 

The energy differences,  $\Delta E = E_{\text{theory}} - E_{\text{NIST}}$ , between the different theoretical excitation energies (M-CDHF, Aggarwal1, Aggarwal2, and Xu) and the NIST compiled values are also reported in Table III. The differences  $\Delta E$  between the present MCDHF/RCI energies and the NIST values deduced from measured lines are well controlled within 2 800 cm<sup>-1</sup>, and are generally within or smaller than the NIST estimated uncertainties. On the contrary, the two theoretical data sets of Aggarwal et al. [8] deviate from the NIST measured values by up to  $\simeq 15~700~\text{cm}^{-1}$ . Moreover, these two data sets do not support each other well, revealing deviations of up to  $\simeq 11~000~\text{cm}^{-1}$ . Similarly, the excitation energies calculated by Xu et al. [9] differ from the NIST measured values by up to 15 000 cm<sup>-1</sup>.

The differences between the previous calculations of atomic energy levels [8, 9] and the NIST measured value are several times or one order of magnitude larger than the corresponding differences calculated for the present theoretical MCDHF/RCI energies. This indicates that the present theoretical excitation energies of S-like W are highly accurate and represent a great improvement on the latest theoretical results [8, 9]. In addition, excitation energies in Table III are presented in the order of the present theoretical excitation energies. The results from the previous calculations [8, 9] that do not correspond to this order are coloured in blue. This explicitly illustrates that the order of the levels from the previous calculations is not always correct, although some levels are very close to each other, in which case the order remains uncertain.

Looking at the NIST values that are reported in square brackets to mark their origin from semi-empirical parametric calculations, their differences with the present theoretical values are usually about tens of thousands  $\rm cm^{-1}$ , with the largest difference of 46 000 cm<sup>-1</sup>. For this reason, our MCDHF/RCI excitation energies, compared with these NIST compiled values, also represent a substantial improvement in accuracy. We therefore recommend the use of the present theoretical values for updating these NIST semi-empirical data, and even suggest their use as input data for a new parametric fit using Cowan's code, which would increase dramatically the accuracy and quality of the NIST compiled values.

Spectroscopists pay close attention to the  $n = 3 \rightarrow n = 3$  transitions of S-like W that can be used as benchmarks for advancing electron-correlation physics in multielectron high-Z ions. Furthermore, the  $n = 3 \rightarrow n = 3$  forbidden transitions, such as 3p - 3p and 3d - 3d, are also important for plasma diagnostics because their line intensity ratios are highly sensitive to the electron den-

sity. We compare in Table IV the present MCDHF/RCI wavelengths with the measured values in the range of 10 Å to 60 Å [1, 2, 40], as well as with previous theoretical values (Aggarwal1, Aggarwal2, and Xu) [8, 9]. The theory-observation deviations  $\Delta \lambda$  (in mÅ) are also listed in the same table. The agreement between the experimental and present theoretical wavelength values is generally within 10 mÅ for the transitions in the X-ray region. This signifies that the accuracy of our calculations is high enough to confirm or revise experimental identifications. For comparison, the results from Ref. [8] and from Ref. [9] deviate from the measured values by up to 130 mÅ and 336 mÅ, respectively. Their differences with the experimental wavelength values are also usually several times or one order of magnitude larger compared with the corresponding MCDHF/RCI differences.

The line at 34.779(4) Å, measured by Lennartsson et al. [2] using the EBIT facility, was not explicitly identified, since relatively limited RCI calculations were available for supporting line assignments. The calculated RCI values for the  $3s^23p^4 \ ^1D_2 \rightarrow 3s^23p^4 \ ^3P_2$  (an M1 transition) and  $3s^23p^3(^2P)3d \ ^1P_1 \rightarrow 3s^23p^4 \ ^3P_2$  (an E1 transition) in Ref. [2], are respectively 34.735 Å, 34.800 Å. They are "equally close" to the measured wavelength of 34.779(4) Å. By comparison, our MCDHF values are, respectively, 34.819 Å and 34.773 Å for these E1 and M1 transitions. Our theoretical wavelength  $\lambda = 34.773$  Å for the M1 transition agrees well enough with the measured wavelength at  $\lambda = 34.779(4)$  Å to suggest to assign the latter to the M1 transition, but not to the E1 transition.

Among the previous different calculations [8, 9], the M1 transitions are not reported in Ref. [9]. Therefore, this theoretical work cannot be used to assign the line 34.779(4) Å due to incomplete data. The results provided in Ref. [8] for these E1 and M1 transitions are, respectively, 34.74 Å and 34.78 Å. By comparison, the present MCDHF/RCI values are respectively 34.819 Å and 34.773 Å, i.e. a wavelength for the E1 transition longer than for the M1 transition. This fact alone illustrates that the order of the  $3s^23p^4$   $^1D_2$  and  $3s^23p^3(^2P)3d$   $^1P_1$  levels found in the calculations [8] is most likely not correct, as pointed out above.

Accurate wavelengths  $(\lambda)$ , transition rates (A), weighted oscillator strengths (gf) and line strengths (S) for E1, E2, M1 and M2 transitions with a radiative branching ratio larger than 0.1 % involving the lowest 88 levels from the present MCDHF/RCI calculations are listed in

Table V. All E1 and E2 transitions are calculated in Babushkin (length) gauge. Compared with the calculations [8], the present theoretical calculations also provide a complete data set of accurate radiative transition data. Aggarwal et al. stated that calculations were performed for the transitions among the lowest 220 levels of the n = 3 configurations, whereas radiative rates were only reported for the transitions involving the two lowest levels (The data involving the higher levels did not belong to S-like W). Future modeling and diagnosing of plasmas would benefit from the present complete data sets of high accuracy. The present work could also be used for cross-checking work under progress [41] on the inclusion of QED corrections in GRASP2018 [42].

#### IV. CONCLUSION

We calculated the energy levels, wavelengths, and E1, E2, M1, and M2 transition parameters among the 88 lowest levels for S-like W using the MCDHF and RCI methods [16] implemented in the GRASP2K package [16, 17]. We analyzed in detail the relative importance of different physical effects, namely, VV and CV electron correlations, the Breit interaction, the higher-order frequencydependent retardation correction through the Transverse Photon interaction, and the QED corrections, using for the latter three different models.

The Breit and QED corrections play an important

role in the calculations of excitation energies and wavelengths in S-like W. The CV electron and the higherorder retardation corrections beyond the Breit interaction, which were not considered in previous calculations [8–11], should not be ignored for getting high-precision results. The present set of results is accurate enough to support and help spectroscopists in their delicate and challenging task of spectral lines identification. We expect that the present complete and accurate atomic data set for S-like W would benefit future modeling and diagnosing of plasmas.

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TABLE I. Excitation energies  $(E, \text{ in cm}^{-1})$  from the present MCDHF/RCI calculations, compared with experimental values compiled in the NIST ASD [14]. The estimated uncertainty of the experimental value for each level is reported in brackets in the  $E_{\text{NIST}}$  column. The MCDHF values were calculated using the Dirac-Coulomb Hamitonian with CSF expansions targeting valence (VV) and core-valence (CV) electron correlation; The DCB and DCTP values were obtained by considering in the RCI step the Dirac-Coulomb-Breit (9) and Dirac-Coulomb-Transverse-Photon (10) Hamiltonians, respectively. The QED corrections were estimated using the three different models (M1-M3)(see the text for details). The differences  $\Delta E = E_{\text{MCDHF/RCI}} - E_{\text{NIST}}$ are also reported (in cm<sup>-1</sup>).

Key			$E_{\mathrm{MCDHI}}$	$_{\rm F}~({\rm cm}^{-1})$		$E_{\rm RCI}$ (	-1)			$\Delta E$	$= E_{MO}$	CDHF/I	RCI - E	NIST (	in cm <sup>-</sup>	•1)
	Level	$E_{\rm NIST}~({\rm cm}^{-1})$	VV	+CV	DCB	DCTP		+QED		VV	$+\mathrm{CV}$	DCB	DCTP		+QED	
							M1	M2	M3					M1	M2	M3
3 6 7 15 27 28 29	$\begin{array}{c} 3s^2 3p^3 (^2 P) 3d \ ^3 D_2^o \\ 3s^2 3p^3 (^2 P) 3d \ ^3 F_0^a \\ 3s^2 3p^3 (^2 P) 3d \ ^3 F_0^a \\ 3s_3 p^5 \ ^3 P_0^a \\ 3s^2 3p^3 (^2 D) 3d \ ^1 F_0^a \\ 3s^2 3p^3 (^2 D) 3d \ ^3 F_2^o \\ 3s^2 3p^3 (^2 D) 3d \ ^3 S_1^o \end{array}$	$\begin{array}{c} 1893900(700)\\ 1966200(800)\\ 2574320(110)\\ 4282700(1800)\\ 4963500(1500)\\ 5018300(2500)\\ 5062800(2100) \end{array}$	$1908452 \\1985487 \\2608264 \\4322043 \\5017897 \\5071977 \\5114885$	$\begin{array}{c} 1906355\\ 1983233\\ 2606644\\ 4320956\\ 5013815\\ 5066689\\ 5109250\\ \end{array}$	$1896235 \\1968900 \\2575895 \\4315574 \\4968599 \\5028431 \\5074042$	$\begin{array}{c} 1900096\\ 1972761\\ 2579342\\ 4311808\\ 4968098\\ 5027550\\ 5073037\end{array}$	$1894013 \\1966720 \\2574485 \\4281212 \\4964990 \\5021539 \\5066102$	$1893744 \\1966449 \\2574205 \\4282365 \\4964223 \\5020965 \\5065599$	$1893519 \\1966226 \\2574094 \\4282846 \\4964236 \\5021025 \\5065679$	14552 19287 33944 39343 54397 53677 52085	$12455 \\ 17033 \\ 32324 \\ 38256 \\ 50315 \\ 48389 \\ 46450 \\$	2335 2700 1575 32874 5099 10131 11242	6196 6561 5022 29108 4598 9250 10237	113 520 165 -1488 1490 3239 3302	-156 249 -115 -335 723 2665 2799	-381 26 -226 146 736 2725 2879

TABLE II: Wavelength deviations  $\Delta\lambda$  (in mÅ) between the present theoretical  $\lambda$ -values calculated in different levels of approximations and the measured values  $\lambda_{exp.}$  (in Å) together with theoretical transition rates A (in  $s^{-1}$ ). The third column specifies the transition mode (TM) considered for the reported rate. For each transition, the estimated uncertainty in the experimental wavelength value is reported in brackets in the  $\lambda_{exp.}$  column. Valence and core-valence electron correlation are included through the MCDHF calculations using the Dirac-Coulomb (DC) Hamiltonian. The DCTP value result from the RCI calculations including the transverse photon interaction, as described in the text. The +QED columns report values obtained by adding the QED(M2) corrections to the DCTP Hamiltonian.

Upper level	Lower level	ТМ	$\lambda_{\rm exp}$ (Å)		$\Delta\lambda$ (mÅ	Å)		$A  ({\rm s}^{-1})$	
			()	DC	DCTP	+ QED	DC	DCTP	+ QED
$3s^2 3p^3(^2D) 3d \ ^3S_1^o$	$3s^2 3p^4 {\ }^3 P_2$	E1	$19.752(8)^a$	-180	-40	-11	4.838E + 12	4.672E + 12	4.737E + 12
$3s^2 3p^3 (^2D) 3d \ ^3P_2^o$	$3s^2 3p^{4-3} P_2$	E1	$19.927(10)^a$	-227	-27	-11	4.201E + 12	4.176E + 12	4.095E + 12
$3s^2 3p^3 (^2D) 3d \ ^1F_3^o$	$3s^2 3p^{4-3} P_2$	E1	$20.147(6)^{a}$	-247	-47	-3	2.981E + 12	2.902E + 12	2.894E + 12
$3s3p^{5-3}P_2^o$	$3s^2 3p^{4-3} P_2$	E1	$23.350(1)^{a}$	-250	-150	2	8.616E + 11	8.090E + 11	8.314E + 11
$3s^2 3p^{4-1} D_2$	$3s^2 3p^{4-3} P_2$	M1	$34.779(4)^{b}$	7	24	-6	2.076E + 08	1.999E + 08	2.004E + 08
$3s^2 3p^3 ({}^{\hat{2}}P) 3d {}^{3}D_3^o$	$3s^2 3p^{4-3} P_2$	$\mathbf{E1}$	$35.974(2)^{b}$	-374	-74	-12	5.293E + 11	5.143E + 11	5.112E + 11
$3s^2 3p^3 (^2P) 3d \ ^1P_1^o$	$3s^2 3p^{4-1} S_0$	E1	$36.881(3)^{b}$	-381	-81	-11	2.814E + 11	2.735E + 11	2.715E + 11
$3s^2 3p^3 (^2P) 3d \ ^3P_2^o$	$3s^2 3p^{4-3} P_2$	$\mathbf{E1}$	$38.072(2)^{b}$	-472	-72	-10	1.486E + 11	1.448E + 11	1.431E + 11
$3s^2 3p^3 (^2P) 3d \ ^3F_3^o$	$3s^2 3p^{4-3} P_2$	$\mathbf{E1}$	$50.86(2)^{c}$	-460	-160	-7	1.741E + 09	1.626E + 09	1.616E + 09
$3s^2 3p^3 ({}^2P) 3d \; {}^3D_2^o$	$3s^2 3p^4 {}^3 P_2$	E1	$52.80(2))^{c}$	-300	-200	5	9.009E + 09	$8.883\mathrm{E}+09$	$8.784\mathrm{E}+09$

 $^a$  From Ralchenko et al. [40]

<sup>b</sup> From Lennartsson et al. [2] <sup>c</sup> From Clementson et al. [1]

TABLE III: Computed excitation energies  $(E, \text{ in cm}^{-1})$  from the present MCDHF/RCI calculations (DCTP Hamiltonian + QED-M2), as well as from the previous theoretical works [8] (Aggarwal1 and Aggarwal2) and [9] (Xu), are compared with the values compiled in the NIST AS-D [14]. The differences ( $\Delta E$ , in cm<sup>-1</sup>) of the different theoretical results and the NIST values are listed along with the present theoretical lifetimes ( $\tau$ , in s). The NIST compiled values reported in square brackets are determined by semi-empirical parametric calculations using Cowan's code. The rest of the NIST values are deduced from measured lines. The number reported in parenthesis, after the NIST excitation energy, is the estimated accuracy provided by the NIST ASD. The results from the previous calculations [8, 9] that do not correspond to this order are marked as bold.

Kev	Level		E (	$(\mathrm{cm}^{-1})$			$\Delta E = I$	$E_{\rm theory}$ –	$E_{\rm NIST}$ (	$(\mathrm{cm}^{-1})$	$\tau$ (s)
		NIST	This work	Aggarwal1	Aggarwal2	Xu	This work	Aggarwal1	Aggarwal2	Xu	( )
1	$3s^23p^{4-3}P_2$	0	0	0	0	0	0	0	0	0	
2	$3s^23p^{4-1}S_0$	[153000](10000)	159769	161215	161040	155262	6769	8215	8040	2262	6.98E - 02
3	$3s^23p^3(^2P)3d^3D_2^o$	1893900(700)	1893744	1897578	1889677	1881974	-156	3678	-4223	-11926	1.14E - 10
4	$3s^2 3p^3 (^2P) 3d \ ^3P_1^{\bar{o}}$	[1959000](20000)	1962235	1966635	1958690		3235	7635	-310		5.08E - 11
5	$3s^2 3p^3 (^2P) 3d \ ^3P_0^{o}$	[1959000](20000)	1964560	1968830	1960885	1954201	5560	9830	1885	-4799	1.48E - 01
6	$3s^2 3p^3 (^2P) 3d \ ^3F_3^o$	1966200(800)	1966449	1971288	1963343	1953805	249	5088	-2857	-12395	6.19E - 10
7	$3s^2 3p^3 (^2P) 3d \ ^3F_4^o$	2574320(110)	2574205	2576171	2568896	2559173	-115	1851	-5424	-15147	3.81E - 07
8	$3s^2 3p^3 (^2P) 3d \ ^3P_2^{o}$	[2627000](30000)	2627280	2629712	2622448	2640103	280	2712	-4552	13103	6.99E - 12
9	$3s^2 3p^3 (^2P) 3d \ ^3D_3^o$	[2775000](30000)	2780684	2786483	2779251	2781879	5684	11483	4251	6879	1.96E - 12
10	$3s^23p^{4}{}^3P_1$	[]()	2798651	2797193	2799772				-		2.17E - 09
11	$3s^23p^3(^2P)3d^{-1}P_1^o$	[2849000](30000)	2871998	2878201	2870904	2873826	22998	29201	21904	24826	3.10E - 12
12	$3s^23n^{4-1}D_2$	[=010000](00000)	2875791	2875524	2877949	_0.00_0		-0-01	-1001	- 10-0	3.41E - 09
13	$3s^23n^2({}^3P)3d^2({}^3F_2) {}^5G_2$		3867430	3877469	3860756						3.53E - 11
14	$3s^23n^2({}^3P)3d^2({}^3P_2) {}^5D_0$		4063197	4074064	4057197						2.50E - 11
15	$3s3n^5 {}^3P_0^0$	4282700(1800)	4282365	4295404	4284562	4276537	-335	12704	1862	-6163	1.16E - 12
16	$3s3n^5 \ ^1P^o$	[4458000](40000)	4450056	4460438	4451395	4500816	-7944	2438	-6605	0100	9.84E - 13
17	$3s^23n^2({}^3P)3d^2({}^3F_2) {}^5G_2$	[1100000](10000)	4580627	4589730	4573577	1000010	1011	2100	0000		3.99E - 12
18	$3s^23n^3(^2D)3d^3F_0^o$	[4656000](50000)	4614513	4615925	4610613		-41487	-40075	-45387		1.09E - 10
19	$3s^23n^3(^4S)3d^{-5}D_0^{\circ}$	[4667000](50000)	4626085	4627392	4622092		-40915	-39608	-44908		7.14E - 11
20	$3e^23n^3(^2D)3d^{-3}D_0^2$	[4675000](50000)	4635782	4640056	4633450		-30218	-3/9//	-41550		2.82E = 12
20 21	$3s^2 3n^2 ({}^1S) 3d^2 ({}^3P_2) {}^3P_2$	[4010000](00000)	4670360	4680582	4664407		-00210	-01011	-41000		350E - 12
21	$3e^23n^3(^2D)3d^3C^0$	[4721000](50000)	4670210	4681745	4676370		11781	30255	44621		2.11E - 11
22	$3s^23n^2({}^3P)3d^2({}^3P_2)^5D_1$	[4721000](50000)	4079219	4001740	4070373		-41701	-09200	-44021		2.11E - 11 3.30E - 12
$\frac{20}{24}$	$3s^2 3n^2 ({}^1S) 3d^2 ({}^1C_2) {}^1C_1$		4711168	4723017	4706875						3.0E = 12 3.10E = 12
24 25	$3e^{2}3n^{3}(^{2}D)3d^{3}C^{0}$	[4700000](50000)	4745000	4740080	4743582		44001	40020	46418		1.47E = 08
20 26	$3s^{2}3p^{3}(^{2}D)3d^{3}F^{o}$	[4790000](50000) [4801000](50000)	4745009	4749080	47455640		-44991 38601	-40920	20260		1.47E = 0.0 2.82F 12
$\frac{20}{97}$	$3s^{2}3p^{3}(^{2}D)3d^{1}F^{o}$	[4063500(1500)]	4064993	4072042	4067084	4073658	703	-55750	-33300		3.02E - 12 3.46F - 13
21 28	$3s^{2}3p^{3}(^{2}D)3d^{3}P^{o}$	4903300(1300) 5018300(2500)	5020065	4973043	5026803	4973030	2665	9040 14484	4404 8503		3.40E = 13 2.44E = 13
20	$3s 3p (D) 3d 1_2$ $3s^2 3n^3 (^2D) 3d ^3 S^o$	5062800(2000)	5065500	5078500	5072377	4903042	2005	15700	0577		2.44E = 13 2.11E = 13
29	$2 a^2 2 a^3 (^2 D) 2 d^3 D^0$	5002800(2100) [5170000](50000)	5160059	5194797	5179099	5144567	2199	14727	9011 9099		2.11E - 13 2.01E - 12
00 91	$2a^{2}2m^{3}(^{2}D)2d^{3}D^{o}$	[5170000](50000)	5109902	5960419	5955791	0144007	-40 27645	14131 90500	42010		2.01E - 13 6.02F 11
01 20	$3s 3p (D) 3u D_3$ $2c^2 2m^3 (4C) 2d^5 D^0$	[5299000](50000)	5201333	5262078	5259761		-37043 95999	-20200	40541		0.92E - 11
ა∠ ეე	$3s 3p (3)3a D_4$ $2s^2 2m^3 (^2D) 2d^3 E^0$	[5299000](50000)	5203100	5205076	5200409		41990	-00922	45190		2.79E = 09
აა 94	$3s  3p  (D) 3u  r_4$ $2  a^2 2  m^2 ({}^1 C) 2  d^2 ({}^3 C)  {}^3 C$	[3400000](30000)	5267176	5276777	5261206		-41260	-40438	-45169		9.71E - 09 2.12F - 12
04 95	$3s  3p  (S) 3a  (F_2)  F_4$ $2a^2 2n^3 (^2D) 2d  ^3C^0$	[5422000](50000)	5200000	5201502	5301200		22010	26109	41160		2.12E - 12
30 96	$3s  3p  (D) 3u  G_5$	[5426000](50000)	5202000	5391392	5360640		-36010	-30408	-41100 22051		1.11E - 0.00
30 27	$3s 3p (5)3a D_1$ $2s^2 2m^3 (^2D) 2d ^1 S^0$	[5420000](50000)	5390009	5390637 E 409010	5380149		-29991	-29145	40000		0.04E - 12
37	$3s 3p^{2}(D)3a S_{0}$	[5447000](50000)	5408130	5408919	5404102		-38870	-38081	-42898		1.15E - 11
38 20	$3s  3p  (P)  3d  (D_2)  F_2$	[5569000](60000)	5442097	0402375 5541200	0430804 5526467		09160	20604	05500		1.70E - 12
39 40	$3s \ 3p \ (5) \ 3a^2 D_2^2$	[0002000](00000)	0000000	0041300	0000407 EE00F0F		-20102	-20094	-20000		4.20E = 11
40	$3s^{-}3p^{-}(^{-}P)3a^{-}F_{3}^{-}$	[502000](60000)	5594869	5598458	0093080 FC010CC		-25131	-21542	-20415		4.99E - 10
41	$3s^{-}3p^{-}(^{-}D)3d^{-}D_{2}^{0}$	[5043000](60000)	3020005	5626024	5021300		-22335	-10976	-21640		1.83E - 12
42	$3s^{-}3p^{-}(^{-}D)3d^{-}P_{1}^{0}$	[5074000](60000)	5649559	0000007	5051505		-24441	-17393	-22495		1.28E - 12
43	$3s 3p (P) 3d^{-} (S_{0}) P_{0}$		3053246	5005277	5049639		00045	00004	07005		1.62E - 12
44	$3s^{-}3p^{\circ}(^{+}S)3d^{\circ}D_{3}^{\circ}$	[5718000](60000)	5688356	5694906	5690165		-29645	-23094	-27835		1.50E - 12

Key	Level	<i>E</i>	$({\rm cm}^{-1})$			$\Delta E$ (	$(\mathrm{cm}^{-1})$		- au (s)
		NIST This work	Aggarwal1	Aggarwal2	Xu	This work Aggarwa	11 Aggarwal2	Xu	
45	$3s^2 3p^3(^2D) 3d \ ^1D_2^o$	[5751000](60000) 5720071	5728804	5723613		-30929 -22196	6 -27387		1.04E - 12
46	$3s^2 3p^{4^{-3}} P_0$	5733781	5732414	5737308					3.23E - 10
47	$3s3p^4(4P)3d\ ^5D_2$	6039589	0 6055667	6037133					3.10E - 12
48	$3s3p^4(4P)3d\ ^5P_1$	6075531	6092341	6073796					2.21E - 12
49	$3s3p^4(4P)3d\ ^5D_3$	6102463	6119776	6101055					2.40E - 12
50	$3s3p^4(4P)3d\ ^3F_4$	6166554	4 6186046	6167160					1.77E - 12
51	$3s3p^4(2S)3d\ ^3D_1$	6290183	6308568	6290066					9.81E - 13
52	$3s3p^4(2P)3d\ ^3P_0$	6362557	6381510	6362800					8.87 E - 13
53	$3s3p^4(2S)3d\ ^3D_2$	6388063	6404204	6387568					1.01E - 12
54	$3s3p^4(2D)3d\ {}^3G_3$	6412456	6433657	6415156					5.61 E - 13
55	$3s3p^4(4P)3d\ {}^5F_1$	6417641	6434437	6417427					1.16E - 12
56	$3s3p^4(2P)3d\ {}^3F_2$	6429402	2 6450228	6431079					8.72E - 13
57	$3s^2 3p^2 ({}^3P) 3d^2 ({}^1D_2) {}^3F_3$	6655158	8 6667562	6652441					7.12E - 13
58	$3s^2 3p^2 ({}^3P) 3d^2 ({}^3F_2) {}^5F_1$	6662143	6679074	6662130					4.56E - 13
59	$3s^2 3p^2 ({}^3P) 3d^2 ({}^3F_2) {}^5F_2$	6675988	8 6695447	6677900					3.34E - 13
60	$3s^2 3p^2 ({}^1D) 3d^2 ({}^3F_2) {}^3H_4$	6694464	4 6706124	6691507					1.20E - 12
61	$3s3p^4(4P)3d\ {}^5F_5$	6704396	$6\ 6720127$	6701844					2.88E - 12
62	$3s3p^4(4P)3d\ ^5D_4$	6728314	4 6744203	6725987					2.07E - 12
63	$3s3p^4(4P)3d\ ^3P_0$	6878106	6895202	6877270					1.78E - 12
64	$3s3p^4(4P)3d\ ^3P_1$	6914978	8 6932666	6914592					1.16E - 12
65	$3s3p^4(4P)3d\ ^3F_3$	6926242	2 6943508	6925621					1.42E - 12
66	$3s^2 3p^2 (^3P) 3d^2 (^3P_2) {}^5P_1$	6960549	0 6977175	6962503					2.79E - 13
67	$3s^2 3p^2 (^1D) 3d^2 (^3F_2) \ ^3F_2$	6981515	6997971	6983782					2.46E - 13
68	$3s3p^4(2P)3d \ ^3F_4$	7030629	0 7047276	7029970					8.87E - 13
69	$3s3p^4(4P)3d\ ^5P_3$	7043764	4 7059215	7045399					2.95E - 13
70	$3s3p^4(2S)3d\ ^3D_3$	7057111	7079868	7060740					2.97 E - 13
71	$3s^2 3p^2 ({}^3P) 3d^2 ({}^3F_2) {}^5D_1$	7057700	) <b>7078079</b>	7063176					1.58E - 13
72	$3s3p^4(4P)3d^{-3}D_2$	7067673	3 7092290	7070331					1.03E - 12
73	$3s^2 3p^2 ({}^1D) 3d^2 ({}^1S_0) {}^1D_2$	7080981	7097206	7086090					2.00 E - 13
74	$3s3p^5 \ ^3P_0^o$	[7141000](70000) 7094887	7104196	7096811		-46113 -36804	4 -44189		7.70E - 13
75	$3s^2 3p^2 (^1D) 3d^2 (^3F_2) {}^3P_0$	7115762	2 7137216	7122182					1.36E - 13
76	$3s3p^4(2P)3d^{-3}D_3$	7121693	3 7141167	7124114					5.86E - 13
77	$3s3p^4(2S)3d^{-1}D_2$	7158298	8 7176985	7159614					1.04E - 12
78	$3s^2 3p^2 ({}^3P) 3d^2 ({}^3F_2) {}^5G_4$	7196198	3 <b>7217588</b>	7188837					3.58E - 12
79	$3s3p^4(4P)3d\ ^3D_1$	7197873	37203212	7200249					6.60 E - 13
80	$3s^2 3p^2 ({}^1D) 3d^2 ({}^3F_2) \; {}^3H_5$	7227799	9 7234235	7220397					9.19E - 11
81	$3s^2 3p^2 ({}^3P) 3d^2 ({}^3P_2)  {}^5D_3$	7240569	0 7248995	7234048					1.88E - 12
82	$3s^2 3p^2 (^3P) 3d^2 (^3P_2) {}^5D_2$	7240809	0 7252912	7238350					$1.24\mathrm{E} - 12$
83	$3s^{2}_{3}3p^{2}(^{3}_{2}P)3d^{2}(^{3}_{2}P_{2}) {}^{5}_{3}S_{2}$	7275238	3 7281839	7268254					5.78E - 12
84	$3s^2 3p^2 ({}^3P) 3d^2 ({}^3P_2) {}^3P_1$	7296416	5 7303688	7289597					3.54E - 12
85	$3s3p^5 \ ^3P_1^o$	[7345000](70000) 7298774	4 7313827	7301372		-46226 -31173	3 -43628		3.82E - 13
86	$3s^{2}3p^{2}(^{3}P)3d^{2}(^{3}P_{2}) \ ^{3}P_{0}$	7307588	3 7315693	7305411					1.49E - 12
87	$3s^{2}_{2}3p^{2}(^{3}_{2}P)3d^{2}(^{3}_{2}F_{2})^{3}_{2}G_{3}$	7334991	7343753	7329783					3.02E - 12
88	$3s^{2}3p^{2}(^{1}D)3d^{2}(^{3}P_{2})^{-3}D_{2}$	7339300	0 7356888	7338815					8.94E - 13

# TABLE III: (continued)

TABLE IV: Comparison of the present MCDHF/RCI (DCTP Hamiltonian + QED-M2) wavelengths with the measured values [1, 2, 40], and with previous theoretical results (Aggarwal1 and Aggarwal2 [8], and Xu [9]). The deviations  $\Delta\lambda$  (in mÅ) of the different theoretical values from the experimental wavelengths are also listed.

Upper level	Lower level	TM		λ	(in Å)				$\Delta\lambda$ (in m	nÅ)	
			Exp.	This work	Aggarwal1	Aggarwal2	Xu	This work	Aggarwal1	Aggarwal2	Xu
$3s^2 3p^3 (^2D) 3d \ ^3S$	$^{o}_{1} 3s^{2}3p^{4} {}^{3}P_{2}$	E1	$19.752(8)^a$	19.741	19.69	19.71		-11	-62	-37	
$3s^2 3p^3 (^2D) 3d ^3P$	$a_{2}^{o} 3s^{2}3p^{4} {}^{3}P_{2}$	E1	$19.927(10)^{a}$	19.916	19.87	19.89	20.15	-11	-57	-34	219
$3s^2 3p^3 (^2D) 3d^{-1}F$	$\frac{1}{3} 3s^2 3p^4 {}^3 P_2$	E1	$20.147(6)^{a}$	20.144	20.11	20.13	20.11	-3	-37	-18	-41
$3s3p^5 \ ^3P_2^o$	$3s^2 3p^4 {}^3 P_2$	E1	$23.350(1)^{a}$	23.352	23.28	23.34	23.38	2	-70	-10	33
$3s^2 3p^{4-1} D_2$	$3s^2 3p^{4} {}^3 P_2$	M1	$34.779(4)^{b}$	34.773	34.78	34.75		-6	1	-32	
$3s^2 3p^3 (^2P) 3d \ ^3D$	${}^{o}_{3} 3s^2 3p^4 {}^{3}P_2$	E1	$35.974(2)^{b}$	35.962	35.89	35.98	35.95	-12	-84	7	-27
$3s^2 3p^3 (^2P) 3d^{-1}P$	$^{o}_{1} 3s^{2}3p^{4-1}S_{0}$	E1	$36.881(3)^{b}$	36.870	36.81	36.90	36.78	-11	-71	21	-97
$3s^2 3p^3 (^2P) 3d \ ^3P$	$^{o}_{2} 3s^{2}3p^{4} {}^{3}P_{2}$	E1	$38.072(2)^{b}$	38.062	38.03	38.13	37.88	-10	-42	60	-195
$3s^2 3p^3 (^2P) 3d \ ^3F$	$a_3^{o} 3s^2 3p^{4-3} P_2$	E1	$50.86(2)^{c}$	50.853	50.73	50.93	51.18	-7	-130	74	322
$3s^2 3p^3 (^2P) 3d \ ^3D$	${}^{o}_{2} 3s^{2}3p^{4} {}^{3}P_{2}$	E1	$52.80(2)^{c}$	52.805	52.70	52.92	53.14	5	-100	119	336

<sup>*a*</sup> From Ralchenko et al. [40],

 $^{b}$  From Lennartsson et al. [2],

 $^{c}$  From Clementson et al. [1].

TABLE V: The present MCDHF/RCI (DCTP Hamiltonian + QED-M2) wavelengths ( $\lambda$ , in Å), transition rates (A, in s<sup>-1</sup>), weighted oscillator strengths (gf, dimensionless), and line strengths (S, in atomic units) for E1, E2, M1, and M2 transitions with radiative branching ratios (BRs) larger than 0.1% among the lowest 88 levels for S-like W. The present Table is published in its entirety in the machine-readable format. The results for the transitions among the 10 lowest levels are shown here for guidance regarding its form and content.

i	i	тм	λ	Α	af	S	BBs
J	1	1 1/1	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	21	91	0	Ditto
2	1	E2	625.90	1.432E + 01	8.409E - 10	1.228E - 03	1.00E + 00
3	1	E1	52.805	8.784E + 09	1.836E - 02	3.192E - 03	1.00E + 00
4	1	E1	50.962	1.452E + 10	1.696E - 02	2.846E - 03	7.40 E - 01
4	2	E1	55.480	5.169E + 09	7.156E - 03	1.307 E - 03	2.63 E - 01
5	1	M2	50.902	6.151E + 00	2.389E - 12	1.410E - 04	8.99 E - 01
5	3	E2	1412.1	1.677 E - 01	5.013E - 11	8.407 E - 04	2.74E - 02
5	4	M1	43013	4.395E - 01	1.219 E - 07	1.297E + 00	7.69 E - 02
6	1	E1	50.853	1.616E + 09	4.387E - 03	7.344E - 04	9.98E - 01
7	1	M2	38.847	2.054E + 04	4.182E - 08	1.097E + 00	7.79 E - 03
7	6	M1	164.54	2.603E + 06	9.508E - 05	3.869E + 00	9.93E - 01
8	1	E1	38.062	1.431E + 11	1.555E - 01	1.948E - 02	1.00E + 00
9	1	E1	35.962	5.112E + 11	6.938E - 01	8.215E - 02	1.00E + 00
10	1	M1	35.732	3.268E + 08	1.877E - 04	1.658E + 00	$7.07\mathrm{E}-01$
10	1	E2	35.732	5.378E + 06	3.088E - 06	8.391E - 04	1.19E - 02
10	2	M1	37.895	1.143E + 08	$7.382 \mathrm{E} - 05$	$6.917\mathrm{E}-01$	$2.47\mathrm{E}-01$
10	3	E1	110.51	1.132E + 06	6.220E - 06	2.263E - 06	$2.17\mathrm{E}-03$
10	4	E1	119.56	7.495E + 06	4.818E - 05	1.896E - 05	1.67 E - 02
10	5	E1	119.89	$6.156\mathrm{E}+06$	3.979E - 05	$1.571\mathrm{E}-05$	1.29E - 02

Note: Only the results for the transitions among the 10 lowest levels are shown here, Table V is available in its entirety

on the *PRA* website.