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 method combined with the relativistic configuration-interaction 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 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 and identification of observed lines in complex spectra.

I. INTRODUCTION

The M-shell ($n = 3$) tungsten ions, such as S-like W^{58+}, 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 and Keenan [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^{-1}. The excitation energies calculated by Xu *et al.* [9] differ by 3000–70 000 cm^{-1} 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, Clementson, and Beiersdorfer [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: $3s^23p^4$ $^1D_2 \rightarrow 3s^23p^4$ $^3P_2$ (an M1 transition of S-like W), $3s^23p^3(^2P)3d$ $^1P_1^o \rightarrow 3s^23p^4$ $^3P_2$ (an E1 transition of S-like W), and $3s^23p^5(^2P)3d^2$ $^4D_{5/2}^o \rightarrow 3s^23p^63d$ $^2D_{3/2}$ (an E1 transition of K-like W), with calculated wavelengths of 34.735 Å, 34.800 Å, and 34.812 Å, respectively [2]. All three wavelengths are "equally close" to the measured one, but all lying outside the experimental error bars of 0.004 Å.

The line at 35.644(4) Å measured by Lennartsson, Clementson, and Beiersdorfer [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^{-1} to 60 000 cm^{-1}, due to the lack of accurate theoretical reference values.

In this paper, using the multiconfiguration 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

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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)

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

The CSFs, $\Phi(\gamma_i PJ)$, are jj-coupled many-electron functions built from antisymmetrized products of one-electron Dirac orbitals, where γ_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

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

and accounts for relativistic kinematic effects.

The configurations $\{3s^2 3p^4,\ 3s^2 3p^2 3d^2,\ 3s 3p^4 3d,\ 3s 3p^2 3d^3,\ 3p^6,\ 3p^4 3d^2\}$ $\{3s^2 3p^3 3d,\ 3s^2 3p 3d^3,\ 3s 3p^5,\ 3s 3p^3 3d^2,\ 3p^5 3d\}$ 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 $n \leqslant 7, l \leqslant 5$ (i.e., up to *h*-orbital symmetry). These CSFs describe the valence-valence (VV) electron correlation. No substitutions were allowed from the 1*s* shell, which defines an inactive closed core. In a second series of calculations we added, to the CSFs above, CSFs resulting from SD-MR substitutions of all the $n = 2, 3$ electrons to $n \leqslant 6,\ l \leqslant 5$, with the restriction of allowing maximum one hole in the $n = 2$ core shell. 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 α^2 approximation, takes the form

$$H_{\mathrm{TP}} = -\sum_{j>i=1}^{N} \left[\frac{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j}{r_{ij}} \cos(\omega_{ij} r_{ij}/c) \right. \\ \left. - (\boldsymbol{\alpha}_i \cdot \boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_j \cdot \boldsymbol{\nabla}_j) \frac{\cos(\omega_{ij} r_{ij}/c) - 1}{\omega_{ij}^2 r_{ij}/c^2} \right], \tag{3}$$

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

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

which is the sum of the Gaunt interaction

$$\mathcal{H}_{\mathrm{Gaunt}} = -\sum_{j>i=1}^{N} \frac{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j}{r_{ij}} \tag{5}$$

and the Breit retardation [22]

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

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

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

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 ω_{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 ω_{ij} can be taken as $\omega_{ij} = \omega_{sr} = -\omega_{qp}$ when the effective potentials are derived "on the energy shell" [16]. Averaging ω_{sr} and ω_{pq} has proved quite effective in bound state calculations involving atomic inner shells for "off-shell" potentials but the individual one-particle energies ϵ_i are physically meaningful only for spectroscopic orbitals. In the present work, the TP Hamiltonian matrix elements therefore include the frequency-dependent contributions when the latter involve the spectroscopic orbitals

$$\{1s_{1/2}, 2s_{1/2}, 2p_{1/2}, 2p_{3/2}, 3s_{1/2}, 3p_{1/2}, 3p_{3/2}, 3d_{3/2}, 3d_{5/2}\}$$

spanning the MR configurations. For contributions involving any of the so-called correlation orbitals that are unoccupied in the MR subspace, but appear in the active orbital sets for describing electron correlation excitations, the low frequency limit $\omega_{ij} \to 0$ is considered.

The current status of bound state quantum electrodynamics calculations of transition energies for a few-electron 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.

(i) 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 [25] and Klarsfeld and Maquet [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].

(ii) 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, Chantler, and Grant [32], is used to evaluate the SE contribution.

(iii) QED-M3. A model QED operator, which also includes the nonlocal QED part to calculate the SE corrections for many-electron atomic systems, was recently developed by Shabaev, Tupitsyn, and Yerokhin (QEDMOD) [33,34]. We also include this model SE operator in the GRASP2K code to evaluate the SE contribution.

For all these three models, only the contribution from the diagonal matrix elements of the QED operator is considered. Further work will quantify the off-diagonal contribution of the QED operator [35]. The last two approaches (QED-M2 and QED-M3) have recently been used for investigating Breit and QED effects in the ground-term fine structures of F-like [36] and Co-like [37] 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 $\mathcal{H}_{DC\,TP}$ 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 CSF 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]. Only the levels for which the NIST compiled values deduced from measured lines are listed in Table I. The atomic units are used throughout the present work, if units are not indicated explicitly. The deviations ($\Delta E = E_{MCDHF/RCI} - E_{NIST}$) 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 ΔE-VV and ΔE-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 $\simeq 1100$–5600 cm^{-1} for the levels considered. This illustrates the importance of core-valence correlation, even for such highly charged ions.

2. 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 $3s^2 3p^3 3d$ configuration by $\simeq 10\,000$–$45\,000$ cm^{-1}. The corresponding effect on the levels arising from the $3s3p^5$ configuration is considerably smaller, around 5000 cm^{-1}.

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

TABLE I. Excitation energies (E, 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_{NIST} column. The MCDHF values were calculated using the Dirac-Coulomb Hamiltonian with CSF expansions targeting valence (VV) and core-valence (CV) electron correlation. The DCB and DC TP 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 $\Delta E = E_{\text{MCDHF-RCI}} - E_{NIST}$ are also reported (in cm⁻¹). The key in the first column is a number assigned to each level, and is available in Table III.

Key	Level	E_{NIST} (cm⁻¹)	E_{MCDHF} (cm⁻¹) VV	+CV	E_{RCI} (cm⁻¹) DCB	DCTP	+QED M1	M2	M3	$\Delta E = E_{\text{MCDHF-RCI}} - E_{NIST}$ (in cm⁻¹) VV	+CV	DCB	DCTP	+QED M1	M2	M3
3	$3s^2 3p^3(^2P)3d\ ^3D_2^o$	1893900(700)	1908452	1906355	1896235	1900096	1894013	1893744	1893519	14552	12455	2335	6196	113	−156	−381
6	$3s^2 3p^3(^2P)3d\ ^3F_3^o$	1966200(800)	1985487	1983233	1968900	1972761	1966720	1966449	1966226	19287	17033	2700	6561	520	249	26
7	$3s^2 3p^3(^2P)3d\ ^3F_4^o$	2574320(110)	2608264	2606644	2575895	2579342	2574485	2574205	2574094	33944	32324	1575	5022	165	−115	−226
15	$3s3p^5\ ^3P_2^o$	4282700(1800)	4322043	4320956	4315574	4311808	4281212	4282365	4282846	39343	38256	32874	29108	−1488	−335	146
27	$3s^2 3p^3(^2D)3d\ ^1F_3^o$	4963500(1500)	5017897	5013815	4968599	4968098	4964990	4964223	4964236	54397	50315	5099	4598	1490	723	736
28	$3s^2 3p^3(^2D)3d\ ^3P_2^o$	5018300(2500)	5071977	5066689	5028431	5027550	5021539	5020965	5021025	53677	48389	10131	9250	3239	2665	2725
29	$3s^2 3p^3(^2D)3d\ ^3S_1^o$	5062800(2100)	5114885	5109250	5074042	5073037	5066102	5065599	5065679	52085	46450	11242	10237	3302	2799	2879

Adding the QED corrections to the MCDHF-RCI excitation energies improves substantially the agreement with observation. These QED corrections reach around 4000–29 000 cm⁻¹. 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 $3s^2 3p^3 3d$ 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 and QED-M3 models lie within the error bars of the estimated experimental uncertainty reported in the E_{NIST} column.

In short, the Breit interaction and QED corrections play the most important role in the calculations of excitation energies of S-like W⁵⁸⁺. 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 high-precision 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 Dirac-Coulomb approximation. Once the $\mathcal{H}_{DC\ TP}$ 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 $-200 \leqslant \Delta\lambda \leqslant +24$ 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 λ_{expt} column. Since the upper and lower levels of the M1 transition $3s^2 3p^4\ ^1D_2 - 3s^2 3p^4\ ^3P_2$ belong to the same configuration, the TP (or Breit) interaction and QED corrections have similar effects on the levels involved, affecting only slightly the wavelength of this intraconfiguration transition.

As far as transition rates are concerned, the magnetic TP interaction decreases transition rates by $\simeq 3\%$, on average.

TABLE II. Wavelength deviations $\Delta\lambda$ (in mÅ) between the present theoretical λ values calculated in different levels of approximations and the measured values λ_{expt} (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 λ_{expt} column. Valence and core-valence electron correlation are included through the MCDHF calculations using the Dirac-Coulomb (DC) Hamiltonian. The DCTP value results 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	TM	λ_{expt} (Å)	$\Delta\lambda$ (mÅ)			A (s^{-1})		
				DC	DCTP	+QED	DC	DCTP	+QED
$3s^2 3p^3(^2D)3d$ $^3S_1^o$	$3s^2 3p^4$ $^3P_2$	E1	19.752(8)[a]	-180	-40	-11	4.838×10^{12}	4.672×10^{12}	4.737×10^{12}
$3s^2 3p^3(^2D)3d$ $^3P_2^o$	$3s^2 3p^4$ $^3P_2$	E1	19.927(10)[a]	-227	-27	-11	4.201×10^{12}	4.176×10^{12}	4.095×10^{12}
$3s^2 3p^3(^2D)3d$ $^1F_3^o$	$3s^2 3p^4$ $^3P_2$	E1	20.147(6)[a]	-247	-47	-3	2.981×10^{12}	2.902×10^{12}	2.894×10^{12}
$3s3p^5$ $^3P_2^o$	$3s^2 3p^4$ $^3P_2$	E1	23.350(1)[a]	-250	-150	2	8.616×10^{11}	8.090×10^{11}	8.314×10^{11}
$3s^2 3p^4$ $^1D_2$	$3s^2 3p^4$ $^3P_2$	M1	34.779(4)[b]	7	24	-6	2.076×10^{8}	1.999×10^{8}	2.004×10^{8}
$3s^2 3p^3(^2P)3d$ $^3D_3^o$	$3s^2 3p^4$ $^3P_2$	E1	35.974(2)[b]	-374	-74	-12	5.293×10^{11}	5.143×10^{11}	5.112×10^{11}
$3s^2 3p^3(^2P)3d$ $^1P_1^o$	$3s^2 3p^4$ $^1S_0$	E1	36.881(3)[b]	-381	-81	-11	2.814×10^{11}	2.735×10^{11}	2.715×10^{11}
$3s^2 3p^3(^2P)3d$ $^3P_2^o$	$3s^2 3p^4$ $^3P_2$	E1	38.072(2)[b]	-472	-72	-10	1.486×10^{11}	1.448×10^{11}	1.431×10^{11}
$3s^2 3p^3(^2P)3d$ $^3F_3^o$	$3s^2 3p^4$ $^3P_2$	E1	50.86(2)[c]	-460	-160	-7	1.741×10^{9}	1.626×10^{9}	1.616×10^{9}
$3s^2 3p^3(^2P)3d$ $^3D_2^o$	$3s^2 3p^4$ $^3P_2$	E1	52.80(2)[c]	-300	-200	5	9.009×10^{9}	8.883×10^{9}	8.784×10^{9}

[a]From Ralchenko *et al.* [41].
[b]From Lennartsson, Clementson, and Beiersdorfer [2].
[c]From Clementson and Beiersdorfer [1].

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 characteristic was also found for the M1 transitions within the $3d^n$ configurations (with $n = 2$–5) in Ref. [38].

C. Comparison with other theoretical works and observation

Excitation energies of S-like W from the present MCDHF-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 and Keenan [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 semiempirical calculations by Kramida [39] using Cowan's code [40]. The other NIST values are deduced from measured lines that were observed using the EBIT facilities [1,41]. For each level, the number reported in parentheses, 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^{-1}, whereas the NIST values deduced by measured lines are much more accurate (110–2500 cm^{-1}).

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

$\simeq 11\,000$ cm^{-1}. Similarly, the excitation energies calculated by Xu *et al.* [9] differ from the NIST measured values by up to 15 000 cm^{-1}.

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 highlighted in boldface. 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 semiempirical parametric calculations, their differences with the present theoretical values are usually about tens of thousands cm^{-1}, with the largest difference of 46 000 cm^{-1}. 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 semiempirical 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

TABLE III. Computed excitation energies (E, 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 ASD [14]. The differences (ΔE, in cm^{-1}) of the different theoretical results and the NIST values are listed along with the present theoretical lifetimes (τ, in s). The NIST compiled values reported in square brackets are determined by semiempirical parametric calculations using Cowan's code. The rest of the NIST values are deduced from measured lines. The number reported in parentheses, after the NIST excitation energy, is the estimated accuracy provided by NIST ASD. The results from the previous calculations [8,9] that do not correspond to this order are highlighted in boldface.

Key	Level	E (cm^{-1})					$\Delta E = E_{\text{theory}} - E_{\text{NIST}}$ (cm^{-1})				τ (s)
		This work	NIST	Aggarwal1	Aggarwal2	Xu	This work	Aggarwal1	Aggarwal2	Xu	
1	$3s^2 3p^4$ $^3P_2$	0	0	0	0	0	0	0	0	0	
2	$3s^2 3p^4$ $^1S_0$	159769	[153000](10000)	161215	161040	155262	6769	8215	8040	2262	6.98×10^{-2}
3	$3s^2 3p^3(^2P)3d$ $^3D_2^o$	1893744	1893900(700)	1897578	1889677	1881974	−156	3678	−4223	−11926	1.14×10^{-10}
4	$3s^2 3p^3(^2P)3d$ $^3P_1^o$	1962235	[1959000](20000)	1966635	1958690		3235	7635	−310		5.08×10^{-11}
5	$3s^2 3p^3(^2P)3d$ $^3P_0^o$	1964560	[1959000](20000)	1968830	1960885	**1954201**	5560	9830	1885	−4799	1.48×10^{-1}
6	$3s^2 3p^3(^2P)3d$ $^3F_3^o$	1966449	1966200(800)	1971288	1963343	**1953805**	249	5088	−2857	−12395	6.19×10^{-10}
7	$3s^2 3p^3(^2P)3d$ $^3F_4^o$	2574205	2574320(110)	2576171	2568896	2559173	−115	1851	−5424	−15147	3.81×10^{-7}
8	$3s^2 3p^3(^2P)3d$ $^3P_2^o$	2627280	[2627000](30000)	2629712	2622448	2640103	280	2712	−4552	13103	6.99×10^{-12}
9	$3s^2 3p^3(^2P)3d$ $^3D_3^o$	2780684	[2775000](30000)	2786483	2779251	2781879	5684	11483	4251	6879	1.96×10^{-12}
10	$3s^2 3p^4$ $^3P_1$	2798651		2797193	2799772						2.17×10^{-9}
11	$3s^2 3p^3(^2P)3d$ $^1P_1^o$	2871998	[2849000](30000)	**2878201**	2870904	2873826	22998	29201	21904	24826	3.10×10^{-12}
12	$3s^2 3p^4$ $^1D_2$	2875791		**2875524**	2877949						3.41×10^{-9}
13	$3s^2 3p^2(^3P)3d^2(^3F_2)$ $^5G_2$	3867430		3877469	3860756						3.53×10^{-11}
14	$3s^2 3p^2(^3P)3d^2(^3P_2)$ $^5D_0$	4063197		4074064	4057197						2.50×10^{-11}
15	$3s3p^5$ $^3P_2^o$	4282365	4282700(1800)	4295404	4284562	4276537	−335	12704	1862	−6163	1.16×10^{-12}
16	$3s3p^5$ $^1P^o$	4450056	[4458000](40000)	4460438	4451395	4500816	−7944	2438	−6605		9.84×10^{-13}
17	$3s^2 3p^2(^3P)3d^2(^3F_2)$ $^5G_3$	4580627		4589730	4573577						3.99×10^{-12}
18	$3s^2 3p^3(^2D)3d$ $^3F_2^o$	4614513	[4656000](50000)	4615925	4610613		−41487	−40075	−45387		1.09×10^{-10}
19	$3s^2 3p^3(^4S)3d$ $^5D_0^o$	4626085	[4667000](50000)	4627392	4622092		−40915	−39608	−44908		7.14×10^{-11}
20	$3s^2 3p^3(^2D)3d$ $^3D_1^o$	4635782	[4675000](50000)	4640056	4633450		−39218	−34944	−41550		2.82×10^{-12}
21	$3s^2 3p^2(^1S)3d^2(^3F_2)$ $^3P_2$	4670360		4680582	4664407						3.50×10^{-12}
22	$3s^2 3p^3(^2D)3d$ $^3G_3^o$	4679219	[4721000](50000)	4681745	4676379		−41781	−39255	−44621		2.11×10^{-11}
23	$3s^2 3p^2(^1S)3d^2(^3P_2)$ $^5D_1$	4708593		4718968	4702760						3.30×10^{-12}
24	$3s^2 3p^2(^1S)3d^2(^1G_2)$ $^1G_4$	4711168		4723017	4706875						3.10×10^{-12}
25	$3s^2 3p^3(^2D)3d$ $^3G_4^o$	4745009	[4790000](50000)	4749080	4743582		−44991	−40920	−46418		1.47×10^{-8}
26	$3s^2 3p^3(^2P)3d$ $^3F_2^o$	4852399	[4891000](50000)	4857270	4851640		−38601	−33730	−39360		3.82×10^{-12}
27	$3s^2 3p^3(^4S)3d$ $^3F_3^o$	4964223	4963500(1500)	4973043	4967984	4973658	723	9543	4484		3.46×10^{-13}
28	$3s^2 3p^3(^2D)3d$ $^3P_2^o$	5020965	5018300(2500)	5032784	5026803	4963842	2665	14484	8503		2.44×10^{-13}
29	$3s^2 3p^3(^2D)3d$ $^3S_1^o$	5065599	5062800(2100)	5078500	5072377		2799	15700	9577		2.11×10^{-13}
30	$3s^2 3p^3(^2D)3d$ $^3D_1^o$	5169952	[5170000](50000)	5184737	5178032	5144567	−48	14737	8032		2.01×10^{-13}
31	$3s^2 3p^3(^2D)3d$ $^3D_3^o$	5261355	[5299000](50000)	5260412	5255781		−37645	−38588	−43219		6.92×10^{-11}
32	$3s^2 3p^3(^4S)3d$ $^5D_4^o$	5263768	[5299000](50000)	5263078	5258459		−35232	−35922	−40541		2.79×10^{-9}
33	$3s^2 3p^3(^2D)3d$ $^3F_4^o$	5364720	[5406000](50000)	5365562	5360811		−41280	−40438	−45189		9.71×10^{-9}
34	$3s^2 3p^2(^1S)3d^2(^3F_2)$ $^3F_4$	5367176		5376777	5361206						2.12×10^{-12}
35	$3s^2 3p^3(^2D)3d$ $^3G_5^o$	5389990	[5428000](50000)	**5391592**	**5386840**		−38010	−36408	−41160		1.11×10^{-8}
36	$3s^2 3p^3(^4S)3d$ $^3D_1^o$	5390009	[5420000](50000)	**5390857**	**5386149**		−29991	−29143	−33851		8.64×10^{-12}

TABLE III. (Continued.)

Key	Level	E (cm^{-1})					$\Delta E = E_{\text{theory}} - E_{\text{NIST}}$ (cm^{-1})				τ (s)
		NIST	This work	Aggarwal1	Aggarwal2	Xu	This work	Aggarwal1	Aggarwal2	Xu	
37	$3s^2 3p^3(^2D)3d\ ^1S_0^o$	[5447000](50000)	5408130	5408919	5404102		−38870	−38081	−42898		1.15×10^{-11}
38	$3s^2 3p^2(^3P)3d^2(^1D_2)\ ^3F_2$		5442097	5452375	5436804						1.76×10^{-12}
39	$3s^2 3p^3(^4S)3d\ ^3D_2^o$	[5562000](60000)	5538838	5541306	5536467		−23162	−20694	−25533		4.25×10^{-11}
40	$3s^2 3p^3(^2P)3d\ ^1F_3^o$	[5620000](60000)	5594869	5598458	5593585		−25131	−21542	−26415		4.99×10^{-10}
41	$3s^2 3p^3(^2D)3d\ ^3D_2^o$	[5643000](60000)	5620665	5626024	5621360		−22335	−16976	−21640		1.83×10^{-12}
42	$3s^2 3p^3(^2D)3d\ ^1P_1^o$	[5674000](60000)	5649559	5656607	**5651505**		−24441	−17393	−22495		1.28×10^{-12}
43	$3s^2 3p^2(^3P)3d^2(^1S_0)\ ^3P_0$		5653246	5665277	**5649639**						1.62×10^{-12}
44	$3s^2 3p^3(^4S)3d\ ^5D_3^o$	[5718000](60000)	5688356	5694906	5690165		−29645	−23094	−27835		1.50×10^{-12}
45	$3s^2 3p^3(^2D)3d\ ^1D_2^o$	[5751000](60000)	5720071	5728804	5723613		−30929	−22196	−27387		1.04×10^{-12}
46	$3s^2 3p^4\ ^3P_0$		5733781	5732414	5737308						3.23×10^{-10}
47	$3s 3p^4(^4P)3d\ ^5D_2$		6039589	6055667	6037133						3.10×10^{-12}
48	$3s 3p^4(^4P)3d\ ^5P_1$		6075531	6092341	6073796						2.21×10^{-12}
49	$3s 3p^4(^4P)3d\ ^5D_3$		6102463	6119776	6101055						2.40×10^{-12}
50	$3s 3p^4(^4P)3d\ ^3F_4$		6166554	6186046	6167160						1.77×10^{-12}
51	$3s 3p^4(^2S)3d\ ^3D_1$		6290183	6308568	6290066						9.81×10^{-13}
52	$3s 3p^4(^2P)3d\ ^3P_0$		6362557	6381510	6362800						8.87×10^{-13}
53	$3s 3p^4(^2S)3d\ ^3D_2$		6388063	6404204	6387568						1.01×10^{-12}
54	$3s 3p^4(^2D)3d\ ^3G_3$		6412456	6433657	6415156						5.61×10^{-13}
55	$3s 3p^4(^4P)3d\ ^5F_1$		6417641	6434437	6417427						1.16×10^{-12}
56	$3s 3p^4(^2P)3d\ ^3F_2$		6429402	6450228	6431079						8.72×10^{-13}
57	$3s^2 3p^2(^3P)3d^2(^1D_2)\ ^3F_3$		6655158	6667562	6652441						7.12×10^{-13}
58	$3s^2 3p^2(^3P)3d^2(^3F_2)\ ^5F_1$		6662143	6679074	6662130						4.56×10^{-13}
59	$3s^2 3p^2(^3P)3d^2(^3F_2)\ ^5F_2$		6675988	6695447	6677900						3.34×10^{-13}
60	$3s^2 3p^2(^1D)3d^2(^3F_2)\ ^3H_4$		6694464	6706124	6691507						1.20×10^{-12}
61	$3s 3p^4(^4P)3d\ ^5F_5$		6704396	6720127	6701844						2.88×10^{-12}
62	$3s 3p^4(^4P)3d\ ^5D_4$		6728314	6744203	6725987						2.07×10^{-12}
63	$3s 3p^4(^4P)3d\ ^3P_0$		6878106	6895202	6877270						1.78×10^{-12}

TABLE III. (Continued.)

Key	Level	E (cm^{-1})					$\Delta E = E_{\text{theory}} - E_{\text{NIST}}$ (cm^{-1})				τ (s)
		NIST	This work	Aggarwal1	Aggarwal2	Xu	This work	Aggarwal1	Aggarwal2	Xu	
64	$3s3p^4(^4P)3d\ ^3P_1$		6914978	6932666	6914592						1.16×10^{-12}
65	$3s3p^4(^4P)3d\ ^3F_3$		6926242	6943508	6925621						1.42×10^{-12}
66	$3s^23p^2(^3P)3d^2(^3P_2)\ ^5P_1$		6960549	6977175	6962503						2.79×10^{-13}
67	$3s^23p^2(^1D)3d^2(^3F_2)\ ^3F_2$		6981515	6997971	6983782						2.46×10^{-13}
68	$3s3p^4(2P)3d\ ^3F_4$		7030629	7047276	7029970						8.87×10^{-13}
69	$3s3p^4(^4P)3d\ ^5P_3$		7043764	7059215	7045399						2.95×10^{-13}
70	$3s3p^4(2S)3d\ ^3D_3$		7057111	7079868	7060740						2.97×10^{-13}
71	$3s^23p^2(^3P)3d^2(^3F_2)\ ^5D_1$		7057700	7078079	7063176						1.58×10^{-13}
72	$3s3p^4(^4P)3d\ ^3D_2$		7067673	7092290	7070331						1.03×10^{-12}
73	$3s^23p^2(^1D)3d^2(^1S_0)\ ^1D_2$		7080981	7097206	7086090						2.00×10^{-13}
74	$3s3p^5\ ^3P^o_0$	[7141000](70000)	7094887	7104196	7096811		−46113	−36804	−44189		7.70×10^{-13}
75	$3s^23p^2(^1D)3d^2(^3F_2)\ ^3P_0$		7115762	7137216	7122182						1.36×10^{-13}
76	$3s3p^4(2P)3d\ ^3D_3$		7121693	7141167	7124114						5.86×10^{-13}
77	$3s^23p^2(2S)3d\ ^1D_2$		7158298	7176985	7159614						1.04×10^{-12}
78	$3s^23p^2(^3P)3d^2(^3F_2)\ ^5G_4$		7196198	7217588	7188837						3.58×10^{-12}
79	$3s3p^4(^4P)3d\ ^3D_1$		7197873	7203212	7200249						6.60×10^{-13}
80	$3s^23p^2(^1D)3d^2(^3F_2)\ ^3H_5$		7227799	7234235	7220397						9.19×10^{-11}
81	$3s^23p^2(^3P)3d^2(^3P_2)\ ^5D_3$		7240569	7248995	7234048						1.88×10^{-12}
82	$3s^23p^2(^3P)3d^2(^3P_2)\ ^5D_2$		7240809	7252912	7238350						1.24×10^{-12}
83	$3s^23p^2(^3P)3d^2(^3P_2)\ ^5S_2$		7275238	7281839	7268254						5.78×10^{-12}
84	$3s^23p^2(^3P)3d^2(^3P_2)\ ^3P_1$		7296416	7303688	7289597						3.54×10^{-12}
85	$3s3p^5\ ^3P^o_1$	[7345000](70000)	7298774	7313827	7301372		−46226	−31173	−43628		3.82×10^{-13}
86	$3s^23p^2(^3P)3d^2(^3P_2)\ ^3P_0$		7307588	7315693	7305411						1.49×10^{-12}
87	$3s^23p^2(^3P)3d^2(^3F_2)\ ^3G_3$		7334991	7343753	7329783						3.02×10^{-12}
88	$3s^23p^2(^1D)3d^2(^3P_2)\ ^3D_2$		7339300	7356888	7338815						8.94×10^{-13}

TABLE IV. Comparison of the present MCDHF-RCI (DCTP Hamiltonian + QED-M2) wavelengths with the measured values [1,2,41], 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 mÅ)			
			Expt.	This work	Aggarwal1	Aggarwal2	Xu	This work	Aggarwal1	Aggarwal2	Xu
$3s^2 3p^3(^2D)3d\ ^3S_1^o$	$3s^2 3p^4\ ^3P_2$	E1	19.752(8)[a]	19.741	19.69	19.71		−11	−62	−37	
$3s^2 3p^3(^2D)3d\ ^3P_2^o$	$3s^2 3p^4\ ^3P_2$	E1	19.927(10)[a]	19.916	19.87	19.89	20.15	−11	−57	−34	219
$3s^2 3p^3(^2D)3d\ ^1F_3^o$	$3s^2 3p^4\ ^3P_2$	E1	20.147(6)[a]	20.144	20.11	20.13	20.11	−3	−37	−18	−41
$3s3p^5\ ^3P_2^o$	$3s^2 3p^4\ ^3P_2$	E1	23.350(1)[a]	23.352	23.28	23.34	23.38	2	−70	−10	33
$3s^2 3p^4\ ^1D_2$	$3s^2 3p^4\ ^3P_2$	M1	34.779(4)[b]	34.773	34.78	34.75		−6	1	−32	
$3s^2 3p^3(^2P)3d\ ^3D_3^o$	$3s^2 3p^4\ ^3P_2$	E1	35.974(2)[b]	35.962	35.89	35.98	35.95	−12	−84	7	−27
$3s^2 3p^3(^2P)3d\ ^1P_1^o$	$3s^2 3p^4\ ^1S_0$	E1	36.881(3)[b]	36.870	36.81	36.90	36.78	−11	−71	21	−97
$3s^2 3p^3(^2P)3d\ ^3P_2^o$	$3s^2 3p^4\ ^3P_2$	E1	38.072(2)[b]	38.062	38.03	38.13	37.88	−10	−42	60	−195
$3s^2 3p^3(^2P)3d\ ^3F_3^o$	$3s^2 3p^4\ ^3P_2$	E1	50.86(2)[c]	50.853	50.73	50.93	51.18	−7	−130	74	322
$3s^2 3p^3(^2P)3d\ ^3D_2^o$	$3s^2 3p^4\ ^3P_2$	E1	52.80(2)[c]	52.805	52.70	52.92	53.14	5	−100	119	336

[a]From Ralchenko *et al.* [41].

[b]From Lennartsson, Clementson, and Beiersdorfer [2].

[c]From Clementson and Beiersdorfer [1].

sensitive to the electron density. We compare in Table IV the present MCDHF-RCI wavelengths with the measured values in the range of 10 Å to 60 Å [1,2,41], 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, Clementson, and Beiersdorfer [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 $3s^2 3p^4\ ^1D_2 \rightarrow 3s^2 3p^4\ ^3P_2$ (an M1 transition) and $3s^2 3p^3(^2P)3d\ ^1P_1 \rightarrow 3s^2 3p^4\ ^3P_2$ (an E1 transition) in Ref. [2], are respectively 34.735 Å and 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 assigning 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 $3s^2 3p^4\ ^1D_2$ and $3s^2 3p^3(^2P)3d\ ^1P_1$ levels

found in the calculations [8] is most likely not correct, as pointed out above.

Accurate wavelengths (λ), 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 [42] on the inclusion of QED corrections in GRASP2018 [43].

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 frequency-dependent 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 higher-order 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

TABLE V. Present MCDHF-RCI (DCTP Hamiltonian + QED-M2) wavelengths (λ, in Å), transition rates (A, in s^{-1}), 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. Only the results for the transitions among the 10 lowest levels are shown here for guidance regarding its form and content. Table V is available in the Supplemental Material [44].

j	i	TM	λ	A	gf	S	BRs
2	1	E2	625.90	1.432×10^1	8.409×10^{-10}	1.228×10^{-3}	1.00×10^0
3	1	E1	52.805	8.784×10^9	1.836×10^{-2}	3.192×10^{-3}	1.00×10^0
4	1	E1	50.962	1.452×10^{10}	1.696×10^{-2}	2.846×10^{-3}	7.40×10^{-1}
4	2	E1	55.480	5.169×10^9	7.156×10^{-3}	1.307×10^{-3}	2.63×10^{-1}
5	1	M2	50.902	6.151×10^0	2.389×10^{-12}	1.410×10^{-4}	8.99×10^{-1}
5	3	E2	1412.1	1.677×10^{-1}	5.013×10^{-11}	8.407×10^{-4}	2.74×10^{-2}
5	4	M1	43013	4.395×10^{-1}	1.219×10^{-7}	1.297×10^0	7.69×10^{-2}
6	1	E1	50.853	1.616×10^9	4.387×10^{-3}	7.344×10^{-4}	9.98×10^{-1}
7	1	M2	38.847	2.054×10^4	4.182×10^{-8}	1.097×10^0	7.79×10^{-3}
7	6	M1	164.54	2.603×10^6	9.508×10^{-5}	3.869×10^0	9.93×10^{-1}
8	1	E1	38.062	1.431×10^{11}	1.555×10^{-1}	1.948×10^{-2}	1.00×10^0
9	1	E1	35.962	5.112×10^{11}	6.938×10^{-1}	8.215×10^{-2}	1.00×10^0
10	1	M1	35.732	3.268×10^8	1.877×10^{-4}	1.658×10^0	7.07×10^{-1}
10	1	E2	35.732	5.378×10^6	3.088×10^{-6}	8.391×10^{-4}	1.19×10^{-2}
10	2	M1	37.895	1.143×10^8	7.382×10^{-5}	6.917×10^{-1}	2.47×10^{-1}
10	3	E1	110.51	1.132×10^6	6.220×10^{-6}	2.263×10^{-6}	2.17×10^{-3}
10	4	E1	119.56	7.495×10^6	4.818×10^{-5}	1.896×10^{-5}	1.67×10^{-2}
10	5	E1	119.89	6.156×10^6	3.979×10^{-5}	1.571×10^{-5}	1.29×10^{-2}

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.

[1] J. Clementson and P. Beiersdorfer, Phys. Rev. A **81**, 052509 (2010).

[2] T. Lennartsson, J. Clementson, and P. Beiersdorfer, Phys. Rev. A **87**, 062505 (2013).

[3] P. Beiersdorfer *et al.*, J. Phys. B: At., Mol., Opt. Phys. **43**, 144008 (2010).

[4] N. J. Peacock, M. G. O'Mullane, R. Barnsley, and M. Tarbutt, Can. J. Phys. **86**, 277 (2008).

[5] C. H. Skinner, Phys. Scr., **T134**, 014022 (2009).

[6] P. Beiersdorfer, J. Clementson, and U. I. Safronova, Atoms **3**, 260 (2015).

[7] J. Rzadkiewicz *et al.*, Phys. Rev. A **97**, 052501 (2018).

[8] K. M. Aggarwal and F. P. Keenan, At. Data Nucl. Data Tables **111-112**, 187 (2016).

[9] M. Xu, A. Yan, S. Wu, F. Hu, and X. Li, Can. J. Phys. **95**, 283 (2017).

[10] P. Quinet, J. Phys. B: At., Mol., Opt. Phys. **44**, 195007 (2011).

[11] G. Singh and N. K. Puri, J. Phys. B: At., Mol., Opt. Phys. **49**, 205002 (2016).

[12] K. G. Dyall, I. P. Grant, C. T. Johnson, F. A. Parpia, and E. P. Plummer, Comput. Phys. Commun. **55**, 425 (1989).

[13] M. F. Gu, Can. J. Phys. **86**, 675 (2008).

[14] A. Kramida, Yu. Ralchenko, J. Reader, and NIST ASD Team, NIST Atomic Spectra Database (ver. 5.5.3), available at https://physics.nist.gov/asd (National Institute of Standards and Technology, Gaithersburg, MD, 2018).

[15] C. Froese Fischer, M. Godefroid, T. Brage, P. Jönsson, and G. Gaigalas, J. Phys. B: At., Mol., Opt. Phys. **49**, 182004 (2016).

[16] I. P. Grant, *Relativistic Quantum Theory of Atoms and Molecules* (Springer Sci. +Bus. Media, LLC, New York, NY, 2007).

[17] P. Jönsson, G. Gaigalas, J. Bieroń, C. Froese Fischer, and I. P. Grant, Comput. Phys. Commun. **184**, 2197 (2013).

[18] I. P. Grant, B. J. McKenzie, P. H. Norrington, D. F. Mayers, and N. C. Pyper, Comput. Phys. Commun. **21**, 207 (1980).

[19] S. Gustafsson, P. Jönsson, C. Froese Fischer, and I. P. Grant, Atoms **5**, 3 (2017).

[20] We would like to stress the importance of the − sign of the second term of (3) inside the brackets. That term is indeed often

wrongly written with a + sign (see, e.g., Ref. [37]). Referring to the original paper by Grant and Pyper [21], the + sign can be used when omitting subscripts i and j of the gradient operators, i.e., involving differentiation with respect to $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ as correctly written in [15].

[21] I. P. Grant and N. C. Pyper, J. Phys. B: At., Mol., Opt. Phys. **9**, 761 (1976).

[22] P. Indelicato, J. P. Santos, S. Boucard, and J.-P. Desclaux, Eur. Phys. J. D **45**, 155 (2007).

[23] P. Indelicato, J. Phys. B: At., Mol., Opt. Phys. **52**, 232001 (2019).

[24] L. W. Fullerton and G. A. Rinker, Phys. Rev. A **13**, 1283 (1976).

[25] P. J. Mohr, At. Data Nucl. Data Tables **29**, 453 (1983).

[26] S. Klarsfeld and A. Maquet, Phys. Lett. B **43**, 201 (1973).

[27] P. J. Mohr and Y. K. Kim, Phys. Rev. A **45**, 2727 (1992).

[28] E. O. Le Bigot, P. Indelicato, and P. J. Mohr, Phys. Rev. A **64**, 052508 (2001).

[29] P. J. Mohr and G. Soff, Phys. Rev. Lett. **70**, 158 (1993).

[30] T. Beier, P. J. Mohr, H. Persson, and G. Soff, Phys. Rev. A **58**, 954 (1998).

[31] T. A. Welton, Phys. Rev. **74**, 1157 (1948).

[32] J. A. Lowe, C. T. Chantler, and I. P. Grant, Radiat. Phys. Chem. **85**, 118 (2013).

[33] V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin, Phys. Rev. A **88**, 012513 (2013).

[34] V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin, Comput. Phys. Commun. **189**, 175 (2015).

[35] C. Y. Zhang *et al.* (unpublished).

[36] M. C. Li, R. Si, T. Brage, R. Hutton, and Y. M. Zou, Phys. Rev. A **98**, 020502(R) (2018).

[37] R. Si, X. L. Guo, T. Brage, C. Y. Chen, R. Hutton, and C. F. Fischer, Phys. Rev. A **98**, 012504 (2018).

[38] M. S. Safronova, U. I. Safronova, S. G. Porsev, M. G. Kozlov, and Yu. Ralchenko, Phys. Rev. A **97**, 012502 (2018).

[39] A. Kramida, Can. J. Phys. **89**, 551 (2011).

[40] R. D. Cowan, Phys. Today **35**(6), 57 (1982).

[41] Yu. Ralchenko, I. N. Draganic, J. N. Tan, J. D. Gillaspy, J. M. Pomeroy, J. Reader, U. Feldman, and G. E. Holland, J. Phys. B: At., Mol., Opt. Phys. **41**, 021003 (2008).

[42] M. Piibeleht, L. F. Pašteka, R. Si, J. Grumer, and P. Schwerdtfeger, New QED operators and updated CI program in GRASP, 2019, Poster presented at the Solvay Workshop on "New Frontiers in Atomic, Nuclear, Plasma and Astrophysics," Brussels (2019), available at: http://www.solvayinstitutes.be/event/workshop/new_frontiers_2019/Abstract_Book_New_Frontiers.pdf.

[43] C. Froese Fischer, G. Gaigalas, P. Jönsson, and J. Bieroń, Comput. Phys. Commun. **237**, 184 (2019).

[44] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevA.101.032509 for Table V.