Study of coupled-cluster correlations on electromagnetic transitions and hyperfine structure constants of W VI

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Abstract
This work presents precise calculations of important electromagnetic transition amplitudes along with details of their many-body correlations using the relativistic coupled-cluster method. Studies of hyperfine interaction constants, useful for plasma diagnostics, with this correlation exhaustive many-body approach, are another important area of this work. The calculated oscillator strengths of allowed transitions, amplitudes of forbidden transitions and lifetimes are compared with the other theoretical results wherever available and they show a good agreement. Hyperfine constants of different isotopes of W VI, presented in this paper, will be helpful in gaining an accurate picture of the abundances of this element in different astronomical bodies.

Keywords: atomic data, correlation, hyperfine

(Some figures may appear in colour only in the online journal)

1. Introduction

Recent EBIT experiments [1] on extreme ultraviolet emission for few-times ionized tungsten has prompted further study of the forbidden transitions in the optical and near-infrared region of plasma diagnostic. The use of tungsten as a plasma facing material has attracted the interest of scientists involved in the use of tokamaks [2–4]. Though tungsten is available in nature as a metal with a body-center cubic structure, the presence of $^{W_{5+}}$ in particular glasses [5] dictates the behavior of the glasses in a magnetic field through the electron paramagnetic resonance (EPR) of the ion. Therefore, precise values for magnetic dipole transitions becomes important here. Recent work [6] has shown the importance of the study of the hyperfine structure constant of this ion for the EPR estimation using crystal field theory. There have been many scientific studies on material containing neutral or ionized tungsten where detailed spectroscopic data of these ions are required [7–9]. These spectroscopic data are mainly aimed towards ionization energies of low-lying fine structure, hyperfine levels and the various transition mechanisms among them.

The recent work of Safronova et al [10] showed that long lived highly ionized atoms can be an excellent candidate for the frequency standard or to study $\alpha$ variation. And the system, considered here, is ideal for infrared ion clock, whose hyperfine levels require a precise estimate. The first excited state of this ion, $5d_{5/2}$, is a metastable state with the ground state, $5d_{3/2}$. Therefore, the lifetime of this metastable state is important as it can be used as a fusion device in a plasma medium [11]. All the forbidden lines among the low lying states of this ion are sensitive to the collisional de-excitations and are indicators of the electron density and temperature in the emission region in the study of astrophysics [12, 13] and laboratory tokamak plasmas [14]. To have the precise excitation energy in a plasma atmosphere, the estimations of hyperfine splittings, in other word hyperfine structure constants of the system, are indispensable. Due to the extremely high lifetimes of the few
isotopes of this element, the spectroscopic study of tungsten and its highly stripped ions may play an important role in the prediction of age and the procedure for the formation and evolution of astronomical bodies [15, 16]. Moreover, technological developments in the area of high-resolution spectrometers have increased the demand for the study of hyperfine structures of the various isotopes of this ion for different astrophysical purposes [17–19]. In comparison with the highly accurate experimental hyperfine splitting results, our theoretical values are able to estimate the precise magnetic moment of a nucleus of W with a non-zero nuclear spin. These moments affect any unpaired electrons associated with the atom which are useful in the study of the EPR properties of W VI in molecules or cluster materials [20, 21].

The excitation energies [22–29], oscillator strengths [30], radiative rates [27–29, 31], autoionization rates [27–29], dielectronic satellite lines [27–30] and dielectronic recombination rates [27–42] of various tungsten ions have been studied in several recent works, both theoretically and experimentally. Safronova et al [30] calculated some of the oscillator strengths of electric dipole transitions of W VI by the relativistic all-order many-body perturbation theory using single and double excitations (SD) of the configuration space. Yoca et al [43] and Migdalek et al [44] calculated the oscillator strengths of a number of transitions of this ion using core polarization augmented relativistic Hartree–Fock method, which they named HFR+CPOL and DF+CP, respectively. All these results motivate us to re-investigate those transitions. Many-body correlations study is very important here as 3d, 4d and 4f are core orbitals. From our earlier papers [45, 46], it is expected that we will get significant effect of pair correlation for these forbidden transitions. Therefore, the discrepancies between the results demand correlation exhaustive relativistic ab initio calculations for allowed and forbidden transitions of W VI. Here we apply the highly correlated coupled-cluster theory [46, 47] on a relativistic platform (RCC) to calculate the various fine parameters of allowed and forbidden transitions as well as the hyperfine structure constants of few low-lying energy levels for this ion.

\[
O_{k}\rightarrow \langle \Psi_{k}\mid \hat{O}\mid \Psi_{l}\rangle = \frac{\langle \Phi_{k}\mid (1 + S_{k}^{z})e^{T}\hat{O}e^{T}(1 + S_{l}^{z})\mid \Phi_{l}\rangle}{\sqrt{\langle \Phi_{k}\mid (1 + S_{k}^{z})e^{T}\mid \Phi_{k}\rangle \langle \Phi_{l}\mid (1 + S_{l}^{z})\mid \Phi_{l}\rangle}} = \frac{1}{N}\left[ \langle \Phi_{k}\mid \hat{O} + (\hat{O}S_{1}^{z} + S_{1}^{z}\hat{O}) + (\hat{O}S_{2}^{z} + S_{2}^{z}\hat{O}) + \cdots \rangle \mid \Phi_{l}\rangle \right].
\]

(2)

2. Theory

A brief introduction of the formalism of our calculations using the coupled-cluster theory is discussed here and the details of the

**Figure 1.** Percentage of correlation and Gaunt contributions to the energy levels. Here numbers in the horizontal axis refer to the different energy states. They are 1 \(\rightarrow\) 5d\(3/2\), 2 \(\rightarrow\) 5d\(5/2\), 3 \(\rightarrow\) 6s\(1/2\), 4 \(\rightarrow\) 6p\(1/2\), 5 \(\rightarrow\) 6p\(3/2\), 6 \(\rightarrow\) 5f\(7/2\), 7 \(\rightarrow\) 5f\(5/2\), 8 \(\rightarrow\) 7s\(1/2\), 9 \(\rightarrow\) 7p\(1/2\), 10 \(\rightarrow\) 7p\(3/2\), 11 \(\rightarrow\) 5f\(9/2\), 12 \(\rightarrow\) 5f\(7/2\), 13 \(\rightarrow\) 8s\(1/2\).

Here we assume that the valence electron occupies the \(v\) orbital of the atom or ion. \(\mid \Phi_{v}\rangle = a_{v}\mid \Phi_{0}\rangle\), where \(\mid \Phi_{v}\rangle\) and \(\mid \Phi_{0}\rangle\) are the Dirac–Fock (DF) wavefunctions for a single-valence open-shell and closed-shell systems, respectively. The operators \(T\) and \(S\) produce single to multiple electron excitations with respect to the reference \(\mid \Phi_{0}\rangle\) and \(\mid \Phi_{v}\rangle\), respectively. However, in this present case, we consider these excitations up to the level of SD only. Some valence triple excitations are also included in the present formalism using a perturbative treatment [45]. Such an approximation of the coupled-cluster theory to generate highly correlated wavefunctions is known as the coupled-cluster with single, double and valence triple excitations method and is well established, as indicated in our earlier works [46, 56–62].

The general matrix element of any arbitrary operator \(\hat{O}\) can be expressed in the framework of the RCC theory as,
contribution of core correlation. The lowest order of the Bruckner pair-correlation effect in these matrix elements is considered by the term $O_{ij} + S_{ij}$. The core polarization effect is calculated from the term $O_{ij} S_{ij} + S_{ii}$. Here the subscripts '1' and '2' indicate the SD, respectively. However, in addition to these, there are other higher-order coupled-cluster terms, such as, $S_{ij} O_{ji} + S_{ii} O_{ii}$ and normalization correction $O_{k_{i-1}} - NO_{k_{i-1}}$ to a wavefunction, which are included in the present theoretical approach. A detailed explanation of the different correlation contributing factors is available in one of our recent paper [47].

The strength of the present coupled-cluster method is that it can account for the electronic correlation for all orders in the perturbation theory [63]. Also, from a theoretical point of view, the presence of non-linear terms make this theory more correlation exhaustive at a particular level of excitation [47]. One of the limitations of the present method is the non-consideration of full triple excitations and other higher (quadruple and so on) excitations. But these contributions, in general, are within the uncertainty of experimental error [64]. Another drawback of the present approach is the truncations of the exponential factors in equation (2) to linear terms only ($e^T = 1 + T$). This can be circumvented by using normal the coupled-cluster method [65], which is beyond the scope of the present paper.

The expression of the oscillator strength and transition probabilities (in s$^{-1}$) for allowed (E1) and forbidden (E2 and M1) transitions are given in [56, 58, 66]. The single-electron reduced matrix elements corresponding to the electric dipole, electric quadrupole and magnetic dipole transition operators are discussed in detail in many references [57, 67, 68]. The lifetime, $\tau_k$, of state $k$ can be calculated by considering all different channels of emissions to the states $i$ from $k$,

$$\tau_k = \frac{1}{\sum A_{k-i}},$$

where $A_{k-i}$ represents the probability of the transition from $k$ to $i$.

The hyperfine energy shift of an atom or ion is given by [61, 63, 69]

$$H_{\text{hs}} \approx \frac{\text{A}}{2} + \frac{1}{2} \frac{3K(K + 1) - 4J(J + 1)I(I + 1)}{2I(2I - 1)2J(2J - 1)} B.$$  (4)

Here $K = F(F + 1) - I(I + 1) - J(J + 1)$. $A$ and $B$ are the two well-known hyperfine structure constants [69]. The constant $A$ is associated with the magnetic dipole moment of the nucleus. The constant $B$ corresponds to the electric
quadrupole moment of the nucleus. The mathematical expressions used to calculate these constants for single valence systems (considering $v$ th orbital is the valence orbital with relativistic quantum number $\kappa_v$) are as follows [68]:

$$A = \mu_N g_I \frac{\langle J|T^1|J \rangle}{(J + 1)(2J + 1)}$$

$$= - \frac{g_I \kappa_v}{j_v (j_v + 1)} \langle \frac{1}{r^2} \rangle \times 13074.7 \text{ MHz}$$

and

$$B = 2eQ \frac{2J(2J - 1)}{\sqrt{(2J + 1)(2J + 2)(2J + 3)}} \frac{\langle J|T^2|J \rangle}{\langle J|T^1|J \rangle}$$

$$= Q \left( \frac{2j_v - 1}{2j_v + 2} \langle \frac{1}{r^2} \rangle \right) \times 234.965 \text{ MHz}$$

where $\mu_N$ is the nuclear magneton, $g_I$ is the nuclear $g$-factor and $Q$ is the quadrupole moment of the nucleus. $T^1$ and $T^2$ are the two operators which depend on the inverse radial powers of all the electronic coordinates [69]. Their single-particle reduced matrix element forms are discussed explicitly in [69].

### 3. Results and discussions

For our calculations of different transitions and hyperfine properties, we consider the Fermi-type of nuclear charge distribution function [70]. The basis-set expansion technique [71] is used here to construct the single-particle DF orbitals, where each radial basis function is considered to have a Gaussian-type form. The radial dependence of these Gaussian functions is determined by optimizing two radial parameters $\alpha_0$ and $\beta$ [71], respectively. In order to find these optimized parameters, we compare the results of expectation values of $(\hat{r})$, $(1/r)$, and energies for the present DF orbitals, as mentioned above, with those corresponding quantities for the DF orbitals obtained using a sophisticated numerical approach in the GRASP92 code [72]. This comparison leads to an extremely good agreement between the corresponding expectation values at $\alpha_0 = 0.00525$ and $\beta = 2.70$, respectively. The number of Gaussian functions considered to generate the DF orbitals of $s$, $p$, $d$, $f$, $g$ and $h$ symmetries are 33, 30, 25, 21 and 20, respectively. However, due to the computational limit, the number of active DF orbitals for the RCC calculations is restricted to 16, 15, 14, 11, and 7, respectively, from the lowest energies of the above mentioned symmetries. Here the selection criteria of the number of active DF orbitals employed in the RCC calculations was decided by the convergence of correlation energy in the closed shell system. In the following discussions, wherever the correlation contribution $\langle \delta_{\text{corr}} \rangle$ is mentioned, it indicates the difference between the RCC and the corresponding DF results.

Figure 1 shows the Coulomb-correlation contributions to the ionization potentials with respect to the RCC results along with its relativistic effect (Gaunt interaction [73, 74]). One can see from the figure that $5s_{21/2}$ states are maximally correlated (around 3.5%). All the other states have correlation contributions within 1.0% to 2.3%. Gaunt contributions to the ionization potential are too small, compared to the correlation contributions. It varies from −0.04% to 0.06% as shown in the figure.

Though we know core polarization contributes majorly in electric dipole ($E_1$) transition amplitudes, in table 1 one can see that pair correlation contributions are significant. Even in a few cases, they are comparable to core polarization effect. This table shows our calculated results at the DF and the RCC levels along with the different correlation contributing factors. The wavelengths are estimated from the excitation energies given by the National Institute of Standards and Technology (NIST) website ($\lambda_{\text{NIST}}$) [75], wherever available. The RCC wavelengths ($\lambda_{\text{RCC}}$) are also calculated theoretically using the present RCC method. The $E_1$ amplitudes are calculated using both the length and velocity gauge forms, and are found to be in good agreement within 8% in average. It is known that the velocity gauge values are less stable compared to the corresponding length gauge values [76], and therefore, the latter gauge values are used commonly for the calculations of astrophysically important parameters, such as, oscillator strengths, transition rates and lifetime. The length gauge values for all the transitions are correlated at the level of 10% or more than that, except the transitions associated with the $7s_{1/2}$ and $8s_{1/2}$ states. Important correlation mechanism, core correlation (Core corr), core polarization (Core pol) and pair correlation (Pair corr) contributions to the total correlation in the different $E_1$ transition amplitudes are also highlighted in
Table 3. Calculated \( E^2 \) transition amplitudes with the different correlation contributing terms (in au). The experimental (\( \lambda_\text{NIST} \)) and RCC (\( \lambda_\text{RCC} \)) wavelengths are presented in A. The ‘Other\(^a\)’ indicates the results obtained from another method.

| Transition | \( \lambda_\text{NIST} \) | \( \lambda_\text{RCC} \) | DF | Core corr | Pair corr | Core pol | \( \xi_\text{corr} \) | RCC | Other\(^a\) |
|------------|----------------|----------------|----|-----------|-----------|-----------|----------------|----|-----------|
| 5d\(_{5/2}\) – 5d\(_{3/2}\) | 11482.4 | 12611.9 | −1.7155 | 0.0103 | 0.0366 | 0.0807 | 0.1231 | −1.5924 | −1.6610 |
| −5g\(_{5/2}\) | 276.1 | 277.5 | 3.0304 | −0.0032 | −0.0700 | −0.0345 | −0.1078 | 2.9226 |
| −6s\(_{1/2}\) | 1259.0 | 1302.0 | 2.9061 | −0.0010 | −0.0966 | −0.0525 | −0.1451 | 2.7610 | 2.8519 |
| −7s\(_{1/2}\) | 358.5 | 360.0 | 0.2351 | 0.0002 | 0.0143 | 0.0300 | 0.0272 | 0.2623 |
| −8s\(_{1/2}\) | 272.3 | −0.1015 | −0.0001 | 0.0131 | −0.0265 | −0.0308 | −0.1323 |
| 5d\(_{5/2}\) – 5f\(_{5/2}\) | 282.9 | 283.7 | −1.0713 | 0.0013 | 0.0036 | 0.0082 | 0.0133 | −1.0580 |
| −5g\(_{9/2}\) | 282.9 | 283.7 | 3.7912 | −0.0045 | −0.0136 | −0.0323 | −0.0517 | 3.7395 |
| −6s\(_{1/2}\) | 1414.0 | 1451.9 | 3.7129 | −0.0029 | −0.0842 | −0.0544 | −0.1390 | 3.5739 | 3.4949 |
| −7s\(_{1/2}\) | 370.1 | 370.6 | 0.3692 | 0.0008 | 0.0549 | 0.0314 | 0.0672 | 0.4364 |
| −8s\(_{1/2}\) | 278.3 | −0.1585 | −0.0005 | −0.0274 | −0.0280 | −0.0447 | −0.2033 |
| 5f\(_{5/2}\) – 5f\(_{5/2}\) | 133511.4 | 151745.1 | −4.5606 | 0.0020 | 0.3269 | 0.0473 | 0.4121 | −4.1484 |
| −6p\(_{1/2}\) | 876.2 | 873.3 | 9.0523 | 0.0008 | −0.4743 | −0.1071 | −0.6326 | 8.4197 |
| −6p\(_{3/2}\) | 1034.7 | 1033.5 | −5.1391 | −0.0010 | 0.2759 | 0.0558 | 0.3627 | −4.7765 |
| −7p\(_{1/2}\) | 2169.7 | 8.8125 | −0.0004 | −0.7028 | 0.0301 | −0.8323 | 7.9802 |
| −7p\(_{3/2}\) | 1833.1 | 4.3931 | −0.0004 | −0.3692 | 0.0183 | −0.4315 | 3.9077 |
| 5f\(_{5/2}\) – 6p\(_{3/2}\) | 1026.8 | 1026.5 | −12.6148 | −0.0022 | 0.6548 | 0.1347 | 0.8544 | −11.7603 |
| −7p\(_{3/2}\) | 1855.6 | 10.6906 | −0.0009 | −0.8479 | 0.0433 | −0.9884 | 9.7023 |
| 5f\(_{5/2}\) – 5g\(_{7/2}\) | 8333333.3 | 8333333.3 | −9.5003 | 0.0000 | 0.2725 | 0.0162 | 0.2981 | −9.2022 |
| 6p\(_{1/2}\) – 6p\(_{3/2}\) | 5719.5 | 5670.0 | 7.3339 | 0.0018 | −0.2834 | −0.1021 | −0.3899 | 6.9439 |
| −7p\(_{3/2}\) | 591.5 | −3.0526 | 0.0009 | 0.0444 | −0.0437 | 0.0599 | −2.9927 |
| 6p\(_{1/2}\) – 7p\(_{1/2}\) | 700.0 | −4.8266 | 0.0008 | 0.0525 | −0.0354 | 0.0805 | −4.7461 |
| −7p\(_{1/2}\) | 660.9 | 4.0170 | −0.0009 | −0.0381 | 0.0411 | −0.0561 | 3.9608 |
| 7p\(_{1/2}\) – 7p\(_{3/2}\) | 11817.5 | −22.7635 | −0.0004 | 0.9392 | 0.0434 | 1.0574 | −21.7061 |

\(^a\) Reference [43].

Table 4. Calculated \( M1 \) transition amplitudes with the different correlation contributing terms (in au). The ‘Other\(^a\)’ indicates the result obtained using another method.

| Transition | DF | Core corr | Pair corr | Core pol | \( \xi_\text{corr} \) | Total | Other\(^a\) |
|------------|----|-----------|-----------|-----------|----------------|------|-----------|
| 5d\(_{5/2}\) – 5d\(_{5/2}\) | −1.54784 | 0.00789 | 0.00040 | −0.00140 | −0.00139 | −1.54924 | −1.55288 |
| 5f\(_{5/2}\) – 5f\(_{5/2}\) | −1.85149 | 0.00064 | 0.00015 | −0.00030 | 0.00097 | −1.85051 |
| 5g\(_{7/2}\) – 5g\(_{9/2}\) | −2.10814 | 0.00001 | 0.00000 | −0.00003 | −0.00008 | −2.10822 |
| 6p\(_{1/2}\) – 6p\(_{3/2}\) | 1.14487 | −0.00047 | −0.00056 | −0.00009 | −0.00061 | 1.14426 |
| −7p\(_{3/2}\) | 0.08089 | −0.00032 | 0.000296 | 0.00021 | 0.00389 | 0.08477 |
| 6p\(_{1/2}\) – 7p\(_{1/2}\) | −0.09400 | −0.00026 | −0.00893 | −0.00036 | −0.00233 | −0.09633 |
| 7p\(_{1/2}\) – 7p\(_{3/2}\) | −1.14243 | 0.00018 | 0.00022 | 0.00004 | 0.00035 | −1.14208 |

Note: the wavelength corresponding to each transition can be found in table 3.

\(^a\) Reference [43].

Table 5. The lifetime (in s) of 5d\(_{5/2}\) and 6n\(_{1/2}\) states. The ‘Other\(^a\)’ indicates the results obtained by other authors.

| State | Our | Other\(^a\) |
|-------|-----|-----------|
| 5d\(_{5/2}\) | 1.40 × 10\(^{-1}\) | 1.40 × 10\(^{-1}\) |
| 6n\(_{1/2}\) | 3.82 × 10\(^{-4}\) | 3.77 × 10\(^{-4}\) |

\(^a\) Reference [43].
Table 6. Hyperfine A constants with different correlation contributing terms (in MHz).

| State   | DF  | Core corr | Pair corr | Core pol | \( \delta_{\text{corr}} \) | RCC  |
|---------|-----|-----------|-----------|----------|-------------------------|-----|
| 5d_{1/2} | 379.50 | 2.10     | 20.33    | 34.76    | 62.06                   | 441.56 |
| 5d_{5/2} | 147.14 | 1.30     | 5.66     | -96.28   | -80.26                  | 66.88 |
| 5f_{1/2} | 16.86  | 1.01     | 3.50     | 5.62     | 13.38                   | 30.24 |
| 5f_{7/2} | 9.42   | 0.47     | 1.83     | -15.57   | -13.60                  | -4.18 |
| 5g_{7/2} | 0.58   | 0.00     | 0.04     | 0.06     | -0.05                   | 0.53  |
| 5g_{9/2} | 0.37   | 0.00     | 0.02     | -0.70    | -0.67                   | -0.30 |
| 6s_{1/2} | 9759.05 | -158.12  | 920.29   | 860.81   | 1564.44                 | 11323.50 |
| 6p_{1/2} | 2343.47 | -29.92   | 265.56   | 222.03   | 454.95                  | 2798.42 |
| 6p_{3/2} | 258.34  | -1.59    | 28.51    | 53.67    | 87.77                   | 346.11 |
| 7s_{1/2} | 4243.79 | -54.02   | 220.91   | 336.70   | 498.22                  | 4742.01 |
| 7p_{1/2} | 1131.38 | -10.82   | 79.28    | 94.87    | 165.08                  | 1296.46 |
| 7p_{3/2} | 129.14  | -0.44    | 10.38    | 23.73    | 41.62                   | 170.76 |
| 8s_{1/2} | 2931.87 | -33.73   | 18.11    | 222.04   | 203.73                  | 3135.59 |

Table 7. Hyperfine B constants with different correlation contributing terms (in MHz).

| State   | DF  | Core corr | Pair corr | Core pol | \( \delta_{\text{corr}} \) | RCC  |
|---------|-----|-----------|-----------|----------|-------------------------|-----|
| 5d_{1/2} | -1958.31 | -38.74   | -105.78  | -287.29  | -427.60                 | -2385.91 |
| 5d_{5/2} | -2321.05 | -50.07   | -89.60   | -477.65  | -607.46                 | -2928.52 |
| 5f_{1/2} | -131.78  | -7.80    | -27.37   | -372.74  | -349.28                 | -481.06 |
| 5f_{7/2} | -153.22  | -8.86    | -29.93   | -445.18  | -419.46                 | -572.68 |
| 5g_{7/2} | -5.66    | -0.08    | -0.38    | -213.43  | -206.36                 | -212.02 |
| 5g_{9/2} | -6.19    | -0.09    | -0.41    | -233.46  | -225.87                 | -232.06 |
| 6p_{1/2} | -3946.23 | 44.64    | -434.43  | -736.07  | -1113.48                | -5059.71 |
| 7p_{1/2} | -1972.79 | 14.65    | -158.56  | -315.91  | -464.47                 | -2437.25 |

as \( 5f_{5/2,7/2} \rightarrow 5g_{7/2,9/2} \) transitions, are comparable with core polarization contributions. The figures in the parentheses show percentage values of the theoretical uncertainties. These uncertainties are calculated by judging the quality of the wavefunctions of the states associated with a \( E1 \) transition where it peaks. A similar strategy is taken for the uncertainty estimates of \( E2 \) transitions (table 3) and hyperfine A constants (table 6).

Table 2 compares our oscillator strength results with the corresponding SD [30], HFR+CPOL [43] and DF+CP values [44]. They all are falling within the vacuum ultra-violet (UV) region of the electromagnetic spectrum except the transitions \( 7s_{1/2} \rightarrow 7p_{1/2,3/2} \), which are in middle UV and near UV region. We calculate these oscillator strength values using our calculated matrix elements and experimental wavelengths from the NIST wherever available and the approaches by others whose calculations are available based on length gauge only. Therefore, differences among the oscillator strengths obtained from the various methods must come from the corresponding \( E1 \) amplitudes. This table shows an overall good agreement in the corresponding oscillator strength values as calculated by the RCC approach and as calculated using other other methods.

The significant pair correlation effect is obvious in table 3, where we present \( E2 \) transition amplitudes along with the corresponding transition wavelengths. These transitions are either falling in the UV or infra-red (IR) regions, apart from the \( 6p_{1/2} \rightarrow 6p_{3/2} \) transition, which emits yellow light. There are a few results for the \( E2 \) transitions in the literature obtained using the HFR+CPOL method [43], which are in agreement with our RCC results. Unlike the \( E1 \) transitions, here pair correlation is very strong in many transitions and in some cases, such as transitions from the \( 5f_{5/2,7/2} \) states, this correlation factor contains the lions share of the total correlation.

The strong \( E2 \) transition amplitudes are estimated for the \( 5f_{5/2} \rightarrow 6p_{1/2} \); \( 7p_{1/2,3/2} \), \( 5f_{7/2} \rightarrow 6p_{3/2} \); \( 7p_{1/2,3/2} \), \( 5g_{7/2} \rightarrow 5g_{9/2} \); \( 6p_{1/2} \rightarrow 6p_{3/2} \) and \( 7p_{1/2,3/2} \). High impact of correlations are observed for the \( 5d_{3/2} \rightarrow 7s_{1/2}; 8s_{1/2}, 5d_{5/2} \rightarrow 7s_{1/2}; 8s_{1/2} \) transitions. These transitions are correlated by about 12%, 30%, 18% and 28%, respectively. The correlation contributions to all the other transitions are less than 10%.

The \( M1 \) transition amplitudes are presented in table 4 along with the different correlation contributions. As expected, our results are consistent with the earlier calculations [45, 57, 58, 77, 78] on these magnetic dipole transitions for other ionic species. The amplitude of \( 5d_{3/2} \rightarrow 5d_{5/2} \) transition for W VI is available in literature using the HFR+CPOL method [43], agreeing with the present result with 0.2%. The strong amplitudes between the fine structure states of same
Table 8. Hyperfine A constants (in MHz) for different isotopes of W VI. The parenthesis indicate mass numbers of the isotopes.

| State   | A(182) | A(183) | A(184) | A(186) |
|---------|--------|--------|--------|--------|
| 5d\(_{\frac{1}{2}}\) | 488.30 | 441.56 | 541.70 | 576.36 |
| 5d\(_{\frac{3}{2}}\) | 73.94  | 66.88  | 82.05  | 87.33  |
| 5f\(_{\frac{5}{2}}\) | 33.44  | 30.24  | 37.09  | 39.46  |
| 5f\(_{\frac{7}{2}}\) | −4.62  | −4.18  | −5.12  | −5.44  |
| 5g\(_{\frac{7}{2}}\) | 0.59   | 0.53   | 0.65   | 0.70   |
| 5g\(_{\frac{9}{2}}\) | −0.33  | −0.30  | −0.37  | −0.39  |

258\(^+\)I\(_{2}\) level are dominated by the DF values and have correlation contributions of less than 0.1\%. Therefore, the DF calculations for the M1 transitions between the fine structure states are excellent approximations of the total.

The lifetimes of the first and second excited states are presented in table 5. Both the lifetimes are calculated using the RCC forbidden transitions (E2 and M1) amplitudes, and corresponding experimental wavelengths were obtained from the NIST. Our calculations show the metastable state 5d\(_{\frac{1}{2}}\) has a lifetime of about 0.14 second which can be verified in the EBIT experiment, [11, 79] therefore, W VI can be a good candidate for a heavy ion storage ring [80]. Since the E2 and M1 matrix elements for the 5d\(_{\frac{1}{2}}\) → 5d\(_{\frac{1}{2}}\) transition have almost the same order in magnitude, the lifetime of the 5d\(_{\frac{1}{2}}\) state is almost controlled by the M1 transition (see equation (2.4) and equation (2.5) of [58] and equation (3) of the present work). Both the HFR+CPOL [43] calculations of lifetimes are in agreement with our corresponding results.

The hyperfine structure constants A and B of W VI with mass number 183 and nuclear spin 1/2, important parameters for laboratory plasma and EPR properties of molecules, are presented in tables 6 and 7, respectively. Also, these constants are important contributors for high resolution spectroscopy. Both these constants are presented with different correlation contributions.

Theoretical uncertainties in the calculated property parameters can be estimated by the quality of the wave functions, in particular where the amplitudes are significant, at the levels of the DF. Along with that, we should consider the contributions from other correlation terms that are not considered in this paper and quantum electro-dynamic effects (totally at most ±2\%). As a result, our estimated maximum uncertainties are ±3\% for the E1 amplitudes and ±6\% for forbidden transitions and hyperfine constants.

4. Conclusion

We have calculated the transition amplitudes of allowed and forbidden transitions for W VI using a highly correlated relativistic coupled-cluster theory. Hyperfine structure A and B constants for few low-lying states for the various isotopes of this element are estimated where comparison could not be achieved due to a lack of theoretical or experimental evidence. The importance of pair correlation in many-body approaches is studied along with a detailed study of core polarization correlation contributions. Good agreements were achieved between the electric dipole matrix elements based on the length gauge and velocity gauge. Our correlation exhaustive many-body approach provides scope to experimentalists to test their up to date technology. The forbidden IR and optical transitions among the fine structure levels of the 5d and 6p terms, respectively, are very important for laser spectroscopy, plasma research and different atomic physics experiments. Our spectroscopic estimations of these allowed and forbidden transition lines mitigate the demand for high resolution data observed from the stellar and interstellar...
medium. Our hyperfine data for various isotopes are also supplement to this.

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