Accurate estimations of electromagnetic transitions of Sn IV for stellar and interstellar media

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ABSTRACT
Here we report on accurate ab initio calculations to study astrophysically important electromagnetic transition parameters among different low-lying states of Sn IV. Our ab initio calculations are based on the sophisticated relativistic coupled-cluster theory, which almost exhausts many important electron correlations. To establish the accuracy of the calculations, we compare our results with the available experiments and estimates the transition amplitudes in length and velocity gauged for ms. Most of these allowed and forbidden transition wavelengths lie in the infrared region, and they can be observed in the different cool stellar and interstellar media. For the improvement of uncertainty, we use experimental energies to the estimations of the above transition parameters. The presented data will be helpful to find the abundances of the ion in different astrophysical and laboratory plasma.

Key words: atomic data, abundances, stellar and interstellar media

1 INTRODUCTION
The spectrum of triply-ionized tin (SnIII+) was first observed by Rao nearly a century ago Rao (1926). Accurate estimations of transition lines of Sn IV have astrophysical interest since their detection in the stellar medium O'Toole (2004); Chayer et al. (2005). Using the Hubble's Space Telescope Imaging Spectrograph (STIS), O'Toole (2004) observed the presence of Sn IV in several sdB and sdOB stars (HZ44, HD4539, HD171558, HD185510, HD205805, FFAqr, Feige48, Feige65, CPD-64°481, PG0342+026, PG1032+406, PG1104+243, PG1219+534, HD149382, Feige66, Ton S227, PHL932, UVO1758+36) in the spectroscopic analysis at temperature ranging from 2200 K to 40000 K. Chayer et al. (2005) detected the presence of Sn IV in the atmosphere of the cool white dwarfs and observed five spectral lines of Sn IV in the ultraviolet (UV) spectra. Proffitt et al. (2001) determined the tin abundance of the early B-main-sequence star AV304 in the small Magellanic cloud (SMC) by using archival STIS/HST G140M spectral data to measure the 1314.54 Å resonance line of Sn IV.

Chemical evaluation models predict that about two thirds of tin-abundance in solar system is produced by the S-process, with most of the remainder due to the r-process Arlandini et al. (1999); Sneden et al. (1996). Sofia et al. (1999) stated that tin is the first element to show a well-determined interstellar gas phase abundance, formed primarily by the main s-process. Both Sn IV and Sn II can be observed in the different scenario of star evolution. The detections of low ionized tin in the spectra of Goddard High Resolution spectrograph (GHRSP) Hobbs et al. (1993) have drawn the attention of precise experimental and/or theoretical works for high precision spectroscopy of these ions. The EUV photo absorption spectra recorded, using the dual laser producing plasma (DLP) technique has promising application in lithography Lysaght et al. (2005). Dunne & O'Sullivan (1992) have given prediction of the strengths of EUV transition lines of Sn IV using similar procedure. The technological advancement of observational instruments even have resolution to identify hyperfine lines, which are signature of relativistic effect in atoms or ions. There have been few experimental works to measure the lifetime of few energy states of Sn IV Andersen et al. (1972); Kernahan et al. (1985); Pinnington et al. (1987). Theoretical calculations of energies of some low-lying states of this ion are also available in literature Migdałek & Garmulewicz (2000); Glowacki & Migdałek (2009); Ryabtsev et al (2006, 2007). To the best of our knowledge, there is no theoretical calculations of atomic properties for Sn IV which accounts correlations exhaustively. Therefore, there is a requirement of the highly correlated relativistic calculations of transition parameters of SN IV in the determination of its abundances at different stellar and interstellar media.

In this paper, we use a non-linear relativistic coupled cluster (RCC) theory Lindgren & Mukherjee (1987); Bishop (1991); Dixit et al. (2007); Dutta & Majumder (2011, 2012, 2016); Bhowmik et al. (2017a,b, 2018) to calculate electro-
magnetically allowed and forbidden transition strength lifetimes and lifetimes of low lying energy states of Sn IV. The theory includes almost all kinds of many body correlations including core correlation, core polarization, pair correlation Dutta & Majumder (2016); Das et al. (2018) with high efficiency.

In section 2, we brief about the RCC method and provide the expressions of the spectroscopic parameters used in this paper. Section 3 compares our calculated results with the experimental and theoretical values extracted from literature, and provide precise spectroscopic data of transition lines of Sn IV, relevant for astrophysical or astronomical observations.

2 THEORY

The RCC theory is a well-established many body theory which accounts the correlation exhaustively. The correlated matrix element of an operator $\hat{O}$ can be represented as fol-

$$\langle \Psi_{k}\hat{O}\Psi_{i}\rangle_{\Psi_{j}} = \frac{\langle \Phi_{k}|\hat{O}_{j}(1 + S_{i})\Phi_{i}\rangle}{\langle \Phi_{k}|\Phi_{j}\rangle_{\Psi_{i}}}$$

(2)

where, the normalization factor $N$ contains overlap matrix $P_{ij} = \langle \Phi_{k}|\Phi_{j}\rangle_{\Psi_{i}}$, and core-correlated operator is defined as $O = e^{r_{2}}\hat{O}e^{r_{2}}$. The subscripts '1' and '2' of open-shell cluster operator represents the single and double excitations. The matrix elements $(OS_{2i} + S_{2j}^{f}\hat{O})$ yield the pair correlation and core polarization, respectively. The description of electric dipole ($E_{1}$), quadrupole ($E_{2}$) and magnetic dipole ($M_{1}$) matrix element with respect to orbitals are available in ref. Dutta & Majumder (2016)

The transition probabilities, $A_{k\rightarrow i}$, of above electromagnetic multipole channels among the atomic states $|\Psi_{k}\rangle$ and $|\Psi_{i}\rangle$ are given by

$$g_{k}\lambda^{2}A_{k\rightarrow i}^{E_{1}} = 2.0261 \times 10^{18}|(i|\hat{O}|k)|^{2},$$

(3)

$$g_{k}\lambda^{2}A_{k\rightarrow i}^{E_{2}} = 1.1199 \times 10^{15}|(i|\hat{O}|k)|^{2},$$

(4)

$$g_{k}\lambda^{2}A_{k\rightarrow i}^{M_{1}} = 2.697 \times 10^{15}|(i|\hat{O}|k)|^{2}.$$  

(5)

Here $\lambda$ is the wave length of transition in Å and degener-

3 RESULTS AND DISCUSSIONS

The quality of correlated wave functions produced by the RCC method is based on the generation of accurate DF orbitals as explained in the previous section. To generate the precise wavefunctions of DF orbitals, we use basis-set expansion approach (Clementi (1990)) in self-consistent field calculations. Here the radial part of each basis considered to have a Gaussian-type orbital (GTO) having even-tempered exponents Huzinaga & Klobukowski (1993) as basis parameters. The optimization of the parameters is performed Roy & Majumder (2015) such that the even-tempered basis DF wave functions over radial extent mostly agree with the DF wave functions obtained using a sophisticated numerical approach, GRASP92 (Parpia et al. (2006)). For s, p, d, p, f, g and h symmetries, we have chosen 16, 15, 15, 11, 8 and 8 active orbitals, respectively, for the RCC calculations out of 33, 30, 28, 25, 21 and 20 DF orbitals. This choice of active orbitals depend upon the convergence of the core correlation energy in the closed shell system (Dixit et al. (2008)). The maximum difference between our RCC excitation energies and NIST Kramida (2017) results occurs for 6s1/2 state, which is around 0.45%, and the average discrepancy between the two results is about 0.3%.

Table 1. shows the electric dipole ($E_{1}$) transition amplitudes in both length and velocity gauge forms Grant (2007); Johnson (2006) along with the comparison between our calculated and NIST Kramida (2017) extracted transition wavelengths. The correlation contributions to each of the matrix elements can be easily found from the difference between the DF and the RCC transition amplitudes in both the gauge forms. Apart from 5s1/2 $\rightarrow 6p_{1/2,3/2}$ transitions, the average correlation contribution is about 5%. Including these two transitions the average correlation contribution becomes 23%. It notifies that the correlations are significant.
to those relatively weaker transitions. The table also shows good agreement between the length and velocity gauge results and the average difference between them is 3.2%. This agreement is one of the uncertainty estimations of our calculated wavefunctions. The consistent improvement of the ratio between these two gauged results further highlight the accuracy of our calculations. This ratio is 1.06 and 1.01 for $5p \rightarrow 5d$ and $5p \rightarrow 6d$ transitions, respectively. Also, table shows 0.96 and 0.95 values of the ratio for $4f \rightarrow 5d$ and $4f \rightarrow 6d$, respectively. Further accuracy can be analyzed by the consistency of the ratios, $20:10:2$ (approximately), of our calculated transition strengths among $2P_{1/2} \rightarrow 2D_{3/2}$, $2P_{1/2} \rightarrow 2D_{1/2}$ and $2P_{3/2} \rightarrow 2D_{3/2}$, respectively Cowan (1981). Most of the $E1$ transitions, presented here, fall in the ultraviolet region of electromagnetic spectrum apart from few and are especially useful in space telescope based astronomy (Goad et al. (2016)). Some of the transitions, $5s_{1/2} \rightarrow 6p_{1/2,3/2}, 6s_{1/2} \rightarrow 6p_{1/2}, 4f_{3/2} \rightarrow 6d_{3/2,5/2}$ and $4f_{7/2} \rightarrow 6d_{5/2}$ belong to visible energy spectrum and can be used in laser spectroscopy.

Near and Mid-infrared observations in Astronomy using space based telescope, Infrared Space Observatory (Kessler (1996) has opened different areas of astrophysical studies in cool region of space, like interstellar medium Feuchtgruber et al. (1997), planetary nebulae Liu et al. (2001).

Table 2. presents such fine structure transition lines of Sn IV. Apart from their astrophysical importance these transitions present different correlation features of many-body formalism. Therefore, we present the forbidden electric quadrupole ($E2$) and magnetic dipole ($M1$) transitions of them. Like, electric dipole transitions, the accuracy of the calculations can be understood from the comparison of estimations using formulations based on length and velocity gauges. In these transitions the difference is on average 5% apart from $5g_{9/2} \rightarrow 5p_{9/2} \rightarrow E2$ transition where we find large discrepancy. In the later case same discrepancy is observed even at the DF level using sophisticated numerical code GRASP92 Parpia et al. (2006), which is not possible to mitigate by any correlated method. Also, our estimation for microwave transition among $4f$ multiplets show good agreement with relativistic configuration interaction calculations by Ding et al. (2012). As expected, the correlation contributions to the fine structure $M1$ transitions are negligible and therefore for these transitions DF results are very good approximation of the RCC values.

In Table 3, we have listed oscillator strengths of $E1$ transitions, calculated with their experimental transition wavelengths. Due to the better stability of the length gauge form of transition matrix elements compared to its velocity gauge form Grant (2007), we have used the former form of $E1$ transition amplitudes to calculate the oscillator strengths. Our calculated results of oscillator strengths are compared with the previously reported theoretical [Glowacki & Migdalek (2009); Cheng & Kim (1979); Migdalek & Garmulewicz (2000); Migdalek & Baylis (1979)] and experimental data [Andersen et al. (1972); Pinnington et al. (1987)]. Table shows excellent agreement of our results for $5s_{1/2} \rightarrow 5p_{1/2,3/2}$ transitions with the calculations of Glowacki & Migdalek (2009) using configuration interaction method based on DF wavefunctions generated with non-integer (CIDF(q)) outermost core shell occupation numbers. They have shown that the contribution of fractional occupancy parameter at the DF level contributes around 20% to the oscillator strengths. Their configuration space is made up with the single and double excitations as well as some triple excitations from ground state to a few low-lying states. But, our present RCC calculations contain a larger active orbital space to exhaust to the correlation contributions. The comparison with the old calculation by Cheng and Kim using relativistic Hartree-Fock method Cheng & Kim (1979) shows the correlation contributions in these evaluations. Migdalek and Baylis performed relativistic Hartree-Fock theory with core polarization using semi-empirically fitted polarization potential Migdalek & Baylis (1979) for few transitions. Migdalek and Garmulewicz reported the oscillator strengths for a few transitions of Sn IV using two different methods Migdalek & Garmulewicz (2000) and they only differ by the treatment of valence-core exchange potential. The superiority of the present RCC method over all other many-body approaches discussed above that former includes all leading order terms corresponding to core polarization, pair correlation, core correlation along with higher-order terms for the transition matrix element calculations Dixit et al. (2007, 2008); Dutta & Majumder (2016); Bhownik et al. (2017b). Our detail study of correlations show that the core polarization has the dominant contribution in the total correlation in the presented $E1$ transition amplitudes. Therefore, our RCC results are in good agreement with all the core polarization augmented DF results. Some of the experimental data of oscillator strengths of $E1$ transitions of Sn IV were previously reported using Beam-foil technique Andersen et al. (1972); Pinnington et al. (1987) and they are seen to agree excellently with our RCC results. There is only disagreement seen for $5p_{1/2} \rightarrow 5d_{5/2}$. According to the suggestion of Cowan (1981), the ratio of the $f$ – values for $5d_{3/2} \rightarrow 5p_{3/2}$, $5d_{3/2} \rightarrow 5p_{3/2}$ and $5d_{5/2} \rightarrow 5p_{3/2}$ transitions should be around $6:5:1$, respectively. Our calculations show this ratio is $4.6:4.5:1$, respectively, and therefore, the Beam-foil experiment by Pinnington et al. (1987) underestimated the $f$-value.

Table 4. presents the transition rates of $E2$ and $M1$ transitions along with the corresponding experimental wavelengths. Most of the presented transitions are either in the ultra-violet or in the infra-red (IR) regions. The transitions which fall in the ultraviolet region are very important, in general, in astronomical observation and plasma research (Saloman (2004); Morgan et al. (1995); Fahy et al. (2007), Morita et al. (2010)). Recent study of forbidden transitions of monovalent atoms and ions by Safronova et al. (2017) suggests the superior advantage of these transitions in numerical areas in physics and engineering, particularly precision measurement of time and fundamental constants. $5d_{3/2} \rightarrow 6s_{1/2}$ transitions may have applications in infrared laser spectroscopy and plasma research Thogersen et al. (1996). Among all the presented $E2$ transitions, $5s_{1/2} \rightarrow 6d_{3/2,5/2}$ transition matrix elements are maximally correlated, approximately 23% and 27%, respectively. All the other presented $E2$ transitions are less than 8% correlated. However, the $M1$ transitions, $5d_{3/2} \rightarrow 6d_{5/2}$ is abnormally correlated (around 82%) due to the large pair correlation effect Dixit et al. (2007, 2008); Bhownik et al. (2017b). As seen from the table, $5s_{1/2} \rightarrow 5d_{3/2,5/2}$ transi-
tions have stronger probability (almost $10^3 \text{s}^{-1}$) compare to other $E2$ transitions. $M1$ transitions which have probabilities more than $10^{-3} \text{s}^{-1}$, are shown in the table.

Since there is no metastable state of this ion, lifetime of the excited states are expected to be like neutral alkali atoms, of the order of nanosecond (ns). In Table 6, we compare the present lifetimes for few low lying states of Sn IV with the theoretical as well as a few experimental results. The life times are calculated using present RCC amplitudes and the experimental wavelengths from the NIST Kramida (2017) to minimize uncertainty due to the transition wavelengths. Andrés-García et al. have used the Griem semi-empirical approach using the COWAN computer code Andres-Garcia et al. (2016). The other theoretical lifetimes calculated by Cheng and Kim Cheng & Kim (1979) and Migdalek and Baylis Migdalek & Baylis (1979) are also presented in the table for comparison. The listed experimental lifetimes of different excited states of Sn IV measured using Beam-foil spectroscopy Pinninig et al. (1987); Kernahan et al. (1985); Andersen et al. (1972) are very close to our RCC lifetimes results apart from $5d_{5/2}$ due to discrepancy of the $5p_{3/2} \rightarrow 5d_{5/2}$ $E1$ transition as discussed in earlier paragraph.

The theoretical uncertainties in the calculated property parameters are evaluated by the quality of the wave functions at the levels of the DF. Also, we consider the uncertainty contributions from other correlation terms, not considered in this work, and quantum electrodynamics effects. Later contributes at most $\pm 2\%$. Therefore, in this work, the maximum uncertainties are $\pm 2.5\%$ and $\pm 2.3\%$ for the allowed and forbidden transition amplitudes, respectively.

4 CONCLUSIONS

This paper presents the transition amplitudes, strengths and rates of astrophysically important allowed and forbidden transitions for the ion Sn IV using a highly correlated relativistic many-body approach. The transitions presented in this paper, are in ultraviolet, visible, infrared and microwave regions. Our calculated estimations of most of these transitions are in good agreements with the available experimental observations and theoretical calculations. The differences in results are explained and further justified with the help of estimations based on the length and velocity gauged forms. The spectroscopic data of the present work will be useful in the estimations of abundance of the ion in the different astronomical bodies, astrophysical plasma, laboratory plasma, specially in stellar and interstellar media. Since some of the transitions are estimated first time in literature, to best of our knowledge, our calculated data may also help to the astronomer to discover the undiscovered lines in astronomical systems.

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Table 1. The electric dipole transition matrix elements (in a.u.) at the DF & the RCC levels of calculations for both length and velocity gauge forms. Also experimental transition wavelengths ($\lambda_{NIST}$) is compared with the same from our RCC calculations ($\lambda_{RCC}$). Wavelengths are in Å unit.

| Transition | $J_i$ | $J_f$ | $\lambda_{RCC}$ | $\lambda_{NIST}$ | Length Gauge | Velocity Gauge |
|------------|------|------|-----------------|-----------------|--------------|----------------|
| $5s \rightarrow 5p$ | 1/2 | 1/2 | 1400.8 | 1347.5 | 1.8671 | 1.5659 | 1.8226 | 1.9090 |
| | 1/2 | 3/2 | 1320.2 | 1314.5 | 2.6433 | 2.2253 | 2.5697 | 2.2536 |
| $5s \rightarrow 6p$ | 1/2 | 1/2 | 507.2 | 505.4 | 0.0812 | 0.1836 | 0.0914 | 0.1682 |
| | 1/2 | 3/2 | 501.8 | 499.9 | 0.0329 | 0.1834 | 0.0512 | 0.1604 |
| $6s \rightarrow 6p$ | 1/2 | 1/2 | 420.54 | 421.73 | 3.6738 | 3.5135 | 3.6283 | 3.4928 |
| | 1/2 | 3/2 | 389.34 | 386.22 | 5.1600 | 4.9406 | 5.0880 | 4.9508 |
| $5p \rightarrow 6s$ | 1/2 | 1/2 | 962.1 | 956.3 | 1.0166 | 1.0120 | 0.9921 | 0.9888 |
| | 3/2 | 1/2 | 1024.5 | 1019.7 | 1.5836 | 1.5645 | 1.5413 | 1.5181 |
| $5p \rightarrow 7s$ | 1/2 | 1/2 | 621.4 | 619.0 | 3.2234 | 3.3226 | 3.1607 | 3.2529 |
| | 1/2 | 1/2 | 597.8 | 595.1 | 0.3093 | 0.3139 | 0.2982 | 0.3073 |
| $5p \rightarrow 5d$ | 1/2 | 3/2 | 1041.4 | 1044.5 | 2.9490 | 2.6038 | 2.8498 | 2.5826 |
| | 3/2 | 3/2 | 1114.9 | 1120.7 | 1.3294 | 1.2778 | 1.2702 | 1.2051 |
| | 3/2 | 5/2 | 1113.1 | 1119.3 | 4.0488 | 3.8140 | 3.8618 | 3.6150 |
| $5p \rightarrow 6d$ | 1/2 | 3/2 | 607.1 | 605.2 | 0.5164 | 0.3863 | 0.4791 | 0.3815 |
| | 3/2 | 3/2 | 631.4 | 630.0 | 2.3877 | 2.5413 | 2.3499 | 2.3157 |
| | 3/2 | 5/2 | 631.2 | 628.7 | 7.1195 | 7.0158 | 7.0037 | 6.0390 |
| $6p \rightarrow 7s$ | 1/2 | 1/2 | 2528.7 | 2514.8 | 2.0992 | 2.0612 | 2.0623 | 2.0253 |
| | 3/2 | 1/2 | 2672.4 | 2660.6 | 3.2234 | 3.1575 | 3.1607 | 3.0923 |
| $6p \rightarrow 6d$ | 1/2 | 3/2 | 2703.6 | 2706.7 | 5.1306 | 4.9242 | 5.0383 | 4.8533 |
| | 3/2 | 3/2 | 2868.6 | 2876.5 | 2.3877 | 2.2918 | 2.3499 | 2.2660 |
| | 3/2 | 5/2 | 2864.2 | 2849.3 | 7.1195 | 6.8566 | 7.0037 | 6.7880 |
| $5d \rightarrow 6p$ | 3/2 | 1/2 | 3154.8 | 3076.2 | 3.0850 | 3.0584 | 2.9315 | 2.9094 |
| | 3/2 | 3/2 | 2956.4 | 2879.7 | 1.3294 | 1.3231 | 1.2702 | 1.2634 |
| | 3/2 | 5/2 | 2969.8 | 2888.5 | 4.0488 | 3.9850 | 3.8618 | 3.7922 |
| $5d \rightarrow 4f$ | 3/2 | 5/2 | 2241.3 | 2221.6 | 5.5646 | 5.1718 | 5.7219 | 5.4041 |
| | 5/2 | 7/2 | 2265.5 | 2229.8 | 6.6731 | 6.1593 | 6.9000 | 6.4668 |
| | 5/2 | 5/2 | 2249.0 | 2226.8 | 1.4933 | 1.3840 | 1.5262 | 1.4361 |
| $4f \rightarrow 6d$ | 7/2 | 5/2 | 4990.7 | 4020.9 | 4.0987 | 3.8654 | 4.3571 | 4.0997 |
| | 5/2 | 3/2 | 4154.7 | 4085.4 | 3.4912 | 3.3390 | 3.6742 | 3.4986 |
| | 5/2 | 5/2 | 4145.6 | 4030.7 | 0.9218 | 0.8897 | 0.9572 | 0.9200 |
| $4f \rightarrow 5g$ | 7/2 | 7/2 | 2107.8 | 2082.7 | 1.3616 | 1.2583 | 1.3579 | 1.2613 |
| | 7/2 | 9/2 | 2107.8 | 2082.7 | 8.0560 | 7.4448 | 8.0346 | 7.4643 |
| | 5/2 | 7/2 | 2122.3 | 2084.9 | 7.0970 | 6.6454 | 7.0793 | 6.6629 |

Table 2. Fine structure transition amplitudes (in a.u.) of Sn IV in DF and RCC level of calculation.

| Transition | $J_i$ | $J_f$ | $O_{DF}^{P}$ | $O_{RCC}^{P}$ | $O_{DF}^{M}$ | $O_{RCC}^{M}$ |
|------------|------|------|--------------|--------------|--------------|--------------|
| $5p \rightarrow 5p$ | 1/2 | 3/2 | 25.4611 | 24.5380 | 24.3819 | 23.4515 |
| $6p \rightarrow 6p$ | 1/2 | 3/2 | 25.4611 | 24.5380 | 24.3819 | 23.4515 |
| $5d \rightarrow 5d$ | 3/2 | 5/2 | 27.7864 | 26.9633 | 27.5002 | 26.6322 |
| $4f \rightarrow 4f$ | 5/2 | 7/2 | 8.7793 | 8.1111 | 7.0339 | 6.8043 |
| $5g \rightarrow 5g$ | 7/2 | 9/2 | 21.4040 | 21.0925 | 9.3823 | 9.0656 |

a => Ding et al. (2012)
Table 3. Comparison of oscillator strengths \((f)\) (in a.u.) of electric dipole transitions between the RCC and other endeavours (experimental and theoretical). RCC results are obtained using experimental wavelength \((\lambda_{NIST})\) as given here in Å unit.

| Transition | \(J_l\) | \(J_u\) | \(\lambda_{NIST}\) | \(f_{RCC}\) | \(f_{Other}\) |
|------------|---------|---------|-------------------|----------|---------|
| 5s \(\rightarrow\) 5p | 1/2 | 1/2 | 1437.5 | 0.259 | 0.307, 0.255, 0.360, 0.243 |
|  &  |  |  | 0.263, 0.241, 0.240, 0.225<sup>a</sup> | 0.260<sup>b</sup>, 0.249<sup>c</sup> |
|  &  | 1/2 | 3/2 | 1314.5 | 0.572 | 0.671, 0.567<sup>d</sup>, 0.764<sup>e</sup>, 0.538<sup>f</sup> |
|  &  |  |  | 0.583<sup>e</sup>, 0.534<sup>f</sup>, 0.535<sup>g</sup>, 0.500<sup>h</sup> | 0.560<sup>i</sup>, 0.640<sup>j</sup> |
| 5s \(\rightarrow\) 6p | 1/2 | 1/2 | 505.4 | 0.010 | - |
|  &  | 1/2 | 3/2 | 499.9 | 0.010 | - |
| 6s \(\rightarrow\) 6p | 1/2 | 1/2 | 4217.3 | 0.445 | - |
|  &  | 1/2 | 3/2 | 3862.2 | 0.960 | - |
| 5p \(\rightarrow\) 6s | 1/2 | 1/2 | 956.3 | 0.163 | 0.165<sup>d</sup>, 0.161<sup>e</sup>, 0.162<sup>f</sup>, 0.159<sup>g</sup> |
|  &  | 3/2 | 1/2 | 1019.7 | 0.182 | 0.185<sup>d</sup>, 0.182<sup>e</sup>, 0.182<sup>f</sup>, 0.180<sup>g</sup> |
|  &  |  |  |  | 0.180<sup>i</sup> |
| 5p \(\rightarrow\) 7s | 1/2 | 1/2 | 595.1 | 0.025 | - |
|  &  | 3/2 | 1/2 | 619.0 | 1.354 | - |
| 6p \(\rightarrow\) 7s | 1/2 | 1/2 | 2514.8 | 0.257 | - |
|  &  | 3/2 | 1/2 | 2660.6 | 0.285 | - |
| 5p \(\rightarrow\) 5d | 1/2 | 3/2 | 1044.5 | 0.986 | 1.180<sup>e</sup>, 0.972<sup>d</sup>, 0.965<sup>e</sup>, 0.963<sup>f</sup> |
|  &  | 3/2 | 3/2 | 1120.7 | 0.111 | 0.088<sup>d</sup>, 0.098<sup>e</sup>, 0.097<sup>f</sup>, 0.096<sup>g</sup> |
|  &  | 3/2 | 5/2 | 1119.3 | 1.005 | 1.069<sup>e</sup>, 0.885<sup>d</sup>, 0.881<sup>e</sup>, 0.878<sup>f</sup>, 0.866<sup>g</sup>, 0.852<sup>h</sup>, 0.630<sup>i</sup> |
| 5p \(\rightarrow\) 6d | 1/2 | 3/2 | 605.2 | 0.036 | - |
|  &  | 3/2 | 3/2 | 630.0 | 0.661 | - |
|  &  | 3/2 | 5/2 | 628.7 | 5.945 | - |
| 6p \(\rightarrow\) 6d | 1/2 | 3/2 | 2706.7 | 1.360 | - |
|  &  | 3/2 | 3/2 | 2876.5 | 0.139 | - |
|  &  | 3/2 | 5/2 | 2849.3 | 1.256 | - |
| 5d \(\rightarrow\) 6p | 3/2 | 3/2 | 3072.6 | 0.231 | - |
|  &  | 3/2 | 3/2 | 2879.7 | 0.046 | - |
|  &  | 5/2 | 3/2 | 2888.5 | 0.278 | - |
| 5d \(\rightarrow\) 4f | 3/2 | 5/2 | 2221.6 | 0.914 | 1.036<sup>e</sup> |
|  &  | 5/2 | 7/2 | 2229.8 | 0.861 | 0.977<sup>e</sup> |
|  &  | 5/2 | 5/2 | 2226.8 | 0.044 | - |
| 4f \(\rightarrow\) 6d | 7/2 | 5/2 | 4029.0 | 0.141 | - |
|  &  | 5/2 | 3/2 | 4085.4 | 0.138 | - |
|  &  | 5/2 | 5/2 | 4030.7 | 0.010 | - |
| 4f \(\rightarrow\) 5g | 7/2 | 7/2 | 2082.2 | 0.029 | - |
|  &  | 7/2 | 9/2 | 2082.3 | 1.011 | 1.100<sup>e</sup> |
|  &  | 5/2 | 7/2 | 2064.9 | 1.072 | 1.135<sup>e</sup> |

*\(a\) \(\Rightarrow\) CIDF method with integer occupation number\([Glowacki & Migdalek (2009)]\).*

*\(b\) \(\Rightarrow\) CIDF(q) method with non-integer occupation number\([Glowacki & Migdalek (2009)]\).*

*\(c\) \(\Rightarrow\) Relativistic Hartree-Fock method \([Cheng & Kim (1979)]\).*

*\(d\) \(\Rightarrow\) DF+CP method\([Migdalek & Garmulewicz (2000)]\).*

*\(e\) \(\Rightarrow\) DX+CP method with SCE model potential \([Migdalek & Garmulewicz (2000)]\).*

*\(f\) \(\Rightarrow\) DX+CP method with CAFEGE model potential \([Migdalek & Garmulewicz (2000)]\).*

*\(g\) \(\Rightarrow\) DX+CP method with HFEGE model potential \([Migdalek & Garmulewicz (2000)]\).*

*\(h\) \(\Rightarrow\) Semiempirical relativistic HartreeFock (DiracFock) results \([Migdalek & Baylis (1979)]\).*

*\(i\) \(\Rightarrow\) Beam-foil technique \([Andersen et al. (1972)]\).*

*\(j\) \(\Rightarrow\) Beam-foil technique \([Pinnington et al. (1987)]\).*

W. P., 1996, Phys. Rev. Lett. 76, 2870
Table 4. DF and RCC transition rate (in s$^{-1}$) of E2 in length gauge ($A_{\text{DF}}^{\text{E2}}$ and $A_{\text{RCC}}^{\text{E2}}$) and M1 ($A_{\text{DF}}^{\text{M1}}$ and $A_{\text{RCC}}^{\text{M1}}$) along with the experimental wavelengths (\(\lambda_{\text{NIST}}\)) in Å. The notation P(Q) for transition rates means $P \times 10^Q$.

| Transition | $J_1$ | $J_2$ | $\lambda_{\text{NIST}}$ | $A_{\text{DF}}^{\text{E2}}$ | $A_{\text{RCC}}^{\text{E2}}$ | $A_{\text{DF}}^{\text{M1}}$ | $A_{\text{RCC}}^{\text{M1}}$ |
|------------|-------|-------|-----------------------|--------------------|------------------------|-------------------|------------------------|
| 5s – 5d    | 1/2   | 3/2   | 604.9                 | 1.0598(+05)        | 9.2311(+04)           |                   |                       |
|            | 1/2   | 5/2   | 604.6                 | 1.0563(+05)        | 9.2260(+04)           |                   |                       |
| 5s – 6d    | 1/2   | 3/2   | 425.9                 | 1.6629(+04)        | 1.2858(+04)           |                   |                       |
|            | 1/2   | 5/2   | 425.3                 | 1.7794(+04)        | 1.2912(+04)           |                   |                       |
| 5p – 6p    | 1/2   | 3/2   | 766.5                 | 1.4222(+04)        | 1.3055(+04)           | 1.6191(+01)       | 1.3863(+01)           |
|            | 3/2   | 1/2   | 821.2                 | 2.8691(+04)        | 2.6272(+04)           | 2.9720(+01)       | 3.4242(+01)           |
| 5p – 4f    | 3/2   | 7/2   | 745.2                 | 9.5768(+04)        | 8.4420(+04)           |                   |                       |
|            | 3/2   | 5/2   | 744.9                 | 2.3232(+04)        | 1.8862(+04)           |                   |                       |
| 6p – 4f    | 3/2   | 7/2   | 9778.1                | 1.2745(+00)        | 1.1060(+00)           |                   |                       |
|            | 3/2   | 5/2   | 9720.6                | 2.9366(-01)        | 2.6202(-01)           |                   |                       |
| 5d – 6s    | 3/2   | 1/2   | 11319.8               | 5.4750(-01)        | 5.1505(-01)           |                   |                       |
|            | 5/2   | 1/2   | 11457.4               | 7.9011(-01)        | 7.3143(-01)           |                   |                       |
| 5d – 7s    | 3/2   | 1/2   | 1382.9                | 1.0096(+03)        | 9.7368(+02)           |                   |                       |
|            | 5/2   | 1/2   | 1384.9                | 1.6291(+03)        | 1.4869(+03)           |                   |                       |
| 5d – 6d    | 3/2   | 3/2   | 1439.0                | 2.7130(+03)        | 2.5876(+03)           |                   |                       |
|            | 3/2   | 5/2   | 1432.2                | 7.7068(+02)        | 7.5189(+02)           | 1.7655(-01)       | 6.1292(-03)           |
| 5d – 5g    | 3/2   | 7/2   | 1075.5                | 4.2270(+04)        | 3.9004(+04)           |                   |                       |
|            | 5/2   | 7/2   | 1076.8                | 4.8024(+03)        | 4.3446(+03)           |                   |                       |
| 6d – 5g    | 3/2   | 7/2   | 4318.7                | 4.7514(+01)        | 4.5416(+01)           |                   |                       |
|            | 5/2   | 9/2   | 4318.8                | 4.7502(+02)        | 4.5402(+02)           |                   |                       |

Table 5. Lifetimes in ns of few low-lying states.

| Level       | present work | other work(experiment) | other work(theory) |
|-------------|--------------|------------------------|--------------------|
| 5p 1/2      | 1.20         | 1.29 ±0.209, 0.74 ±0.409 | 1.03^a, 0.95^a, 0.89^a |
| 5p 3/2      | 0.90         | 0.81±0.15^a, 0.93±0.23^b, 1.00±0.10^c     | 0.79^d, 0.74^e, 0.68^f |
| 5d 1/2      | 0.28         | 0.34±0.04^a, 0.35±0.03^b                  | 0.23^d, 0.26^e, 0.33^f |
| 5d 3/2      | 0.28         | 0.45±0.05^a, 0.41±0.03^b                  | 0.30^d, 0.29^e, 0.35^f |

^a⇒ Pinnington et al. (1987), ^b⇒ Kernahan et al. (1985), ^c⇒ Andersen et al. (1972)
^d⇒ Andrés-García et al. (2016) ^e⇒ [Cheng & Kim (1979)], ^f⇒ [Migdalek & Baylis (1979)]