Sc III Spectral Properties of Astrophysical Interest

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Transition properties such as oscillator strengths, transition rates, branching ratios and lifetimes of many low-lying states in the doubly ionized scandium (Sc III) are reported. A relativistic method in the coupled-cluster framework has been employed to incorporate the electron correlation effects due to the Coulomb interaction to all orders by considering all possible singly and doubly excited electronic configurations conjointly with the leading order triply excited configurations in a perturbative approach. Present results are compared with the previously reported results for the transition lines of astrophysical interest. In addition, some of the transition properties and lifetimes of few low-lying states are given for the first time. Role of the correlation effects in the evaluation of the transition strengths are described concisely.

I. INTRODUCTION

The low-lying energy spectra of the doubly ionized scandium (Sc III) have been studied precisely [1–4], however accurate results for other transition properties which are of astrophysical interest are almost rarely investigated. Sc is one of the important elements available in the photosphere of the sun [5–8]. With the accurate information of the spectroscopic data of Sc and its ions, one can acquire palpable knowledge about the abundance of this element in the solar photosphere [6, 7]. Abundances of different elements in the sun was studied latest by Anders et al [9], but the Sc abundance is not well known yet in its photosphere. In that context, precise spectroscopic data of Sc or its ions may be helpful for this purpose. These data can also serve as reference to determine abundances of other elements in the metal-poor stars [6]. From the variation study of the Sc abundance pattern in the long lived F- and G- type stars with different metallicity, it is possible to probe the nucleosynthesis and chemical evolution of the elements in our Galaxy [6, 8]. Ambiguity in the finding of the overabundant of Sc in most of the metal rich stars [10] can be resolved from its improved spectroscopic data. It is also known that the collisional de-excitations of the metastable states are rather slow which can lead to build-up of a population of metastable levels due to M1 and E2 forbidden transitions both in the astrophysical objects and primarily, in the low-density laboratory tokamak plasmas [11]. Intensities of these transitions are vital to infer knowledge about the plasma temperature and dynamics which are of crucial quantities for the determination of the electron density and temperature diagnostics in many astronomical objects and in the laboratory tokamak plasmas [11].

Sc III belongs to the potassium (K I) isoelectronic sequence, but their energy level schemes are different. Since Sc III is an ionized atomic system with heavier nucleus than K I, it is expected that the orbitals of this ion are more contracted towards the nucleus than the latter. Therefore, the electron correlation effects can be different in both the systems and the relativistic effects in Sc III can be larger. Only a few rigorous calculations of transition rates, oscillator strengths and lifetimes in a number of states in Sc III are available till date and most of them are just using the mean-field theories. These theoretical, also observed in few cases, transition properties of Sc III can be found in [12–16], out of which our previous reported results on the transition rates and lifetimes of the 3d and 4s states in this ion [16] were the latest. We had evaluated these quantities by calculating the forbidden transition amplitudes using the relativistic coupled-cluster (RCC) method; an all order perturbative relativistic many-body approach. In the present work, we employ the same method but account a large number of configuration interaction space to determine various transition properties of many low-lying states in the considered ion. This method has also been employed successfully in other systems to study these properties very accurately [17–19]. Some of the Sc data through all the stages of ionization are being tabulated by Wiese and Fuhr [20] few decades ago and the corresponding Sc III data can be replaced by the results obtained from the present study for their uses in other applications; especially in the astrophysics.

The remaining part of the paper is organized as follows: In the next section we describe the necessity of the oscillator strengths and lifetimes for astrophysical studies along with the definitions of these quantities for different multipole channels. Then we pursue with presenting and discussing the results in the following section before

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summarizing them.

II. THEORY AND METHOD OF CALCULATIONS

The emission coefficient from an upper level k to the lower level i in a given element for its diagnostic in an astronomical object is given by [21]

$$I_{ki} = \frac{2\pi he^2}{m_e} \frac{g_i f_{ik}}{\lambda_{ki}} \frac{n}{u} \exp(-E_k/k_B T), \qquad (2.1)$$

where λ_{ki}, f_{ik}, g_i, E_k, n, u and T are the wavelength, absorption oscillator strength, statistical weight of the lower level, energy of the upper level, particle density, partition function of an atom or ion and excitation temperature, respectively. In the above expression h, e, m_e and k_B are the universal constants. Therefore, accurate values of f_{ik} are necessary in order to identify the emission coefficients I_{ki} from different objects. It is also possible that f_{ik} can be extracted from the precisely observed I_{ki} values and compared them with the reported results to demonstrate the potency of the employed method. Moreover, the temperature of an astrophysical object can be determined by plotting $ln\left(\frac{I_{ki} \times \lambda_{ki}^3}{g_i f_{ik}}\right)$ against the E_k values [21].

In the macroscopic mechanical equilibrium and with the knowledge of the gas density, the optical depth of the stellar atmosphere can be found by [22]

$$\tau_{\lambda_{ki}} = \int_0^\infty d^3 r \mathcal{V}_i \phi_{\lambda_{ki}} \frac{\pi e^2}{m_e c} f_{ik} \rho_i, \qquad (2.2)$$

where $\mathcal{V}_i$ is the volume density in the state i, $\phi_{\lambda_{ki}}$ is the spectral line profile which can be obtained from the stellar atmosphere and ρ_i is the gas density in the state i, respectively. Accurate values of the oscillator strengths are also necessary for this purpose.

The emission (absorption) oscillator strength f_{ki} (f_{ik}) is given by [23]

$$f_{ki} = 1.4992 \times 10^{-16} A_{ki} \frac{g_k}{g_i} \lambda_{ki}^2 \qquad (2.3)$$

where λ_{ki} and the transition rate A_{ki} are used in Å and s^{-1}, respectively. Sometime the weighted oscillator strengths are commonly used which are obtained from the relation

$$g_i f_{ik} = -g_k f_{ki}, \qquad (2.4)$$

with $g_i = (2J_i + 1)$, for J being the angular momentum of the state.

The transition rates due to E1, E2 and M1 channels

are given by

$$A_{ki}^{E1} = \frac{64\pi^4 e^2 a_0^2}{3h\lambda_{ki}^3 g_k} = \frac{2.02613 \times 10^{18}}{\lambda_{ki}^3 g_k} S_{ki}^{E1} \qquad (2.5)$$

$$A_{ki}^{E2} = \frac{64\pi^6 e^2 a_0^4}{15h\lambda_{ki}^5 g_k} = \frac{1.11995 \times 10^{18}}{\lambda_{ki}^5 g_k} S_{ki}^{E2} \qquad (2.6)$$

and

$$A_{ki}^{M1} = \frac{64\pi^4 e^2 a_0^2 (\alpha/2)^2}{3h\lambda_{ki}^3 g_k} = \frac{2.69735 \times 10^{13}}{\lambda_{ki}^3 g_k} S_{ki}^{M1}, \qquad (2.7)$$

respectively, where we are not accounting the transition rates due to the $M2$ and $E3$ channels for their negligible magnitudes. In the above expressions, units of A_{ki} and λ_{ki} are maintained with Eq. (2.3) and the line strengths are given in atomic unit (a.u.) for the corresponding channel O which are defined as $S_{ki}^O = |\langle J_k||O||J_i\rangle|^2$.

The lifetime of a given state is estimated by taking reciprocal of the total transition rates due to all possible channels O; i.e. the lifetime of the state k is given by

$$\tau_k = \frac{1}{\sum_{O,i} A_{ki}^O}. \qquad (2.8)$$

Similarly, the branching ratio of a given transition in the channel O from a state k to a lower state i is given by

$$\Gamma_{ki}^O = \frac{A_{ki}^O}{\sum_{O,i} A_{ki}^O}$$
$$= \tau_k A_{ki}^O. \qquad (2.9)$$

The considered ion Sc III has the ground state configuration as $[3p^6]\, 3d_{3/2}$ which can be separated into a closed-shell configuration $[3p^6]$ with the valence electron $3d_{3/2}$. By replacing $3d_{3/2}$ valence orbital with any excited state orbital in the above configuration, the corresponding single excited states of this ion can be obtained. In a Fock space representation, we assume a Fermi vacuum as $|\Phi_0\rangle = [3p^6]$ and a reference state with a valence orbital v as $|\Phi_v\rangle = a_v^\dagger|\Phi_0\rangle$ to define different level of excitations. In this approach, it is customary to express the atomic state function (ASF) in the (R)CC framework as (e.g. see [17, 24])

$$|\Psi_v\rangle = e^T\{1 + S_v\}|\Phi_v\rangle, \qquad (2.10)$$

where T and S_v represent the excitation operators carrying the core-core and core-valence electron correlation effects, respectively. In this work, we consider all possible single and double excitations to determine the amplitudes for the T and S_v operators and also the important triple excitations are considered perturbatively in a self-consistent procedure only for the determination of the S_v operator amplitudes; this approach is known generally as the (R)CCSD(T) method. Since Sc III is a medium size atomic system, the CCSD(T) method can be able to incorporate the correlation effects in this ion comprehensively so that the results can be obtained to the required precision.

Excitation amplitudes for T operators are determined using the equation

$$\langle\Phi_0^*|\{\widehat{He^T}\}|\Phi_0\rangle = 0, \qquad (2.11)$$

where $|\Phi_0^*\rangle$ represents all possible singly and doubly excited states with respect to $|\Phi_0\rangle$. After obtaining these solutions, we obtain both the attachment energy ΔE_v (negative of the ionization potential (IP)) and S_v amplitudes simultaneously for a given ASF of configuration $[3p^6]$ with a valence electron denoted by v using the equation

$$\begin{aligned}\langle\Phi_v^L|\{\widehat{He^T}\}\{1+S_v\}|\Phi_v\rangle &= \langle\Phi_v^L|1+S_v|\Phi_v\rangle \times \\ &\quad \langle\Phi_v|\{\widehat{He^T}\}\{1+S_v\}|\Phi_v\rangle \\ &= \langle\Phi_v^L|\delta_{L,v}+S_v|\Phi_v\rangle\Delta E_v,(2.12)\end{aligned}$$

where the superscript L represents for the singly ($L=1$) and doubly ($L=2$) excited hole-particle states. The Dirac-Coulomb Hamiltonian has been considered for the present calculations.

The transition matrix element for a given channel O from state k to state i is evaluated by calculating the expression

$$\frac{\langle\Psi_k|O|\Psi_i\rangle}{\sqrt{\langle\Psi_k|\Psi_k\rangle\langle\Psi_i|\Psi_i\rangle}} = \frac{\langle\Phi_k|\{1+S_k^\dagger\}\overline{O}\{1+S_i\}|\Phi_i\rangle}{\sqrt{\mathcal{N}_k\mathcal{N}_i}} (2.13)$$

where $\overline{O}=e^{T^\dagger}Oe^T$ and $\mathcal{N}_v=\langle\Phi_v|\{1+S_v^\dagger\}\overline{N}\{1+S_v\}|\Phi_v\rangle$ with $\overline{N}=e^{T^\dagger}e^T$. These terms involve non-truncating series and their evaluation procedure is explained elsewhere, e.g. see [17, 24].

The trial DF wave function $|\Phi_0\rangle$ is constructed initially using 32 Gaussian type orbitals (GTOs) for each angular momentum symmetry before obtaining the self-consistent solutions. To obtain the RCC wave functions, we have considered interaction space within 15s, 15p, 15d, 13f and 12g orbitals in contrast to 13s, 12p, 12d, 7f and 5g orbitals in our previous work [16].

III. RESULTS AND DISCUSSIONS

We present first the IP results of various states from this work using the DF and CCSD(T) methods and compare them in Table I with the corresponding values given in the NIST database [25]. The differences between the CCSD(T) results and the NIST data are given as Δ in percentage in the same table. As seen in the table, the differences between these results are sub-one per cent for all the states; in fact, most of the calculated results are within half per cent accurate. Amount of the correlation effects in these results annexed through the CCSD(T) method can be ascertained from the differences between the DF and CCSD(T) results. Agreement between the experimental results quoted in NIST database and CCSD(T) results signify capability of the method for obtaining the correct results in the considered system.

TABLE I: Ionization potentials of different states. Differences between the CCSD(T) and NIST results are given as Δ.

State	DF (cm^{-1})	CCSD(T) (cm^{-1})	NIST [25] (cm^{-1})	Δ (%)
$3d\ ^2D_{3/2}$	186268.97	199168.89	199677.64	0.25
$3d\ ^2D_{5/2}$	186104.28	198916.43	199479.73	0.28
$4s\ ^2S_{1/2}$	168567.35	174283.19	174138.05	0.08
$4p\ ^2P_{1/2}$	133649.63	137631.36	137573.07	0.04
$4p\ ^2P_{3/2}$	133205.60	136139.57	137099.19	0.70
$4d\ ^2D_{3/2}$	50110.93	87392.72	87419.75	0.03
$4d\ ^2D_{5/2}$	50089.33	87290.26	87374.42	0.10
$5s\ ^2S_{1/2}$	83029.85	84743.04	84814.89	0.08
$5p\ ^2P_{1/2}$	70102.15	71481.95	71570.25	0.12
$5p\ ^2P_{3/2}$	69932.66	71299.70	71394.22	0.13
$4f\ ^2F_{5/2}$	61959.64	62707.34	62803.50	0.15
$4f\ ^2F_{7/2}$	61960.23	62707.42	62803.25	0.15
$5d\ ^2D_{3/2}$	33000.09	51366.41	51547.34	0.35
$5d\ ^2D_{5/2}$	32986.18	51342.51	51527.23	0.36
$6s\ ^2S_{1/2}$	49524.46	50238.20	50483.34	0.79
$6p\ ^2P_{1/2}$	43206.41	43837.69	44187.59	0.79
$6p\ ^2P_{3/2}$	43126.91	43752.33	44102.17	0.79

Although the calculated IP results seem to be accurate enough for considering them in the *ab initio* determination of the transition properties, but it can be noticed that the errors associated in the energies get augmented in the estimation of the excitation energies (EEs); particularly between the fine structure states. This is because of the expected non-negligible contribution from other higher relativistic corrections from the QED and Breit interactions which are not considered in the present work. In contrast to the energies, the QED and Breit interaction contributions are known to be small in the estimation of the transition amplitudes. To minimize the uncertainties, we use the experimental energies/wavelengths in the determination of other transition properties.

In Table II, we give the transition matrix elements including their transition strengths due to the E1, M1 and E2 channels; other higher order multiple channel contributions are very small to be neglected here. These results can also be used to estimate the polarizabilities of different states of the considered ion. As seen from the above table, among the forbidden transitions the E2 transition amplitudes are generally significant except between the fine structure transitions where the M1 transition amplitudes are also large enough to be accounted for. Role of the correlation effects to determine these properties can be realized from the differences between the DF and CCSD(T) results given in the same table. Typically the magnitudes of the amplitudes obtained using the CCSD(T) method are smaller compared to the the DF results except where the results are minuscule. This cognition would be pertinent while we compare our tran-

sition rates, oscillator strengths, branching ratios and lifetimes against the earlier reported results which are obtained using the mean-field theory calculations.

TABLE II: Calculated transition amplitudes and line strengths are given in a.u. for different channels.

Transition $i \to f$		Dirac-Fock	CCSD(T)	$S_{i \to f}$
$3d\ ^2D_{5/2}$	$\xrightarrow{M1} 3d\ ^2D_{3/2}$	1.549	1.541	2.37
	$\xrightarrow{E2} 3d\ ^2D_{3/2}$	1.934	1.649	2.72
$4s\ ^2S_{1/2}$	$\xrightarrow{M1} 3d\ ^2D_{3/2}$	~ 0	-0.001	~ 0
	$\xrightarrow{E2} 3d\ ^2D_{3/2}$	4.051	3.589	12.88
	$\xrightarrow{E2} 3d\ ^2D_{5/2}$	4.975	4.414	19.48
$4p\ ^2P_{1/2}$	$\xrightarrow{E1} 3d\ ^2D_{3/2}$	1.535	1.325	1.76
	$\xrightarrow{E1} 4s\ ^2S_{1/2}$	2.584	2.345	5.50
$4p\ ^2P_{3/2}$	$\xrightarrow{E1} 3d\ ^2D_{3/2}$	0.683	0.589	0.35
	$\xrightarrow{E1} 3d\ ^2D_{5/2}$	-2.054	-1.780	3.17
	$\xrightarrow{E1} 4s\ ^2S_{1/2}$	-3.650	-3.318	11.01
	$\xrightarrow{M1} 4p\ ^2P_{1/2}$	-1.154	-1.154	1.33
	$\xrightarrow{E2} 4p\ ^2P_{1/2}$	-12.452	-11.713	137.19
$4d\ ^2D_{3/2}$	$\xrightarrow{M1} 3d\ ^2D_{3/2}$	0.0002	0.0003	~ 0
	$\xrightarrow{E2} 3d\ ^2D_{3/2}$	-2.811	-2.544	6.47
	$\xrightarrow{M1} 3d\ ^2D_{5/2}$	-0.002	-0.006	~ 0
	$\xrightarrow{E2} 3d\ ^2D_{5/2}$	-1.848	-1.678	2.82
	$\xrightarrow{M1} 4s\ ^2S_{1/2}$	~ 0	~ 0	~ 0
	$\xrightarrow{E2} 4s\ ^2S_{1/2}$	-10.102	-9.707	94.22
	$\xrightarrow{E1} 4p\ ^2P_{1/2}$	-3.907	-3.719	13.83
	$\xrightarrow{E1} 4p\ ^2P_{3/2}$	1.758	1.673	2.80
$4d\ ^2D_{5/2}$	$\xrightarrow{M1} 3d\ ^2D_{3/2}$	0.001	0.002	~ 0
	$\xrightarrow{E2} 3d\ ^2D_{3/2}$	1.837	1.662	2.76
	$\xrightarrow{M1} 3d\ ^2D_{5/2}$	0.0005	0.009	~ 0
	$\xrightarrow{E2} 3d\ ^2D_{5/2}$	-3.689	-3.350	11.22
	$\xrightarrow{E2} 4s\ ^2S_{1/2}$	-12.365	-11.882	141.18
	$\xrightarrow{E1} 4p\ ^2P_{3/2}$	5.270	5.018	25.18
	$\xrightarrow{M1} 4d\ ^2D_{3/2}$	1.549	1.548	2.40
	$\xrightarrow{E2} 4d\ ^2D_{3/2}$	16.140	14.972	224.16
$5s\ ^2S_{1/2}$	$\xrightarrow{M1} 3d\ ^2D_{3/2}$	~ 0	~ 0	~ 0
	$\xrightarrow{E2} 3d\ ^2D_{3/2}$	-0.683	-0.514	0.26
	$\xrightarrow{E2} 3d\ ^2D_{5/2}$	0.844	0.643	0.41
	$\xrightarrow{M1} 4s\ ^2S_{1/2}$	~ 0	-0.002	~ 0
	$\xrightarrow{E1} 4p\ ^2P_{1/2}$	-1.453	-1.442	2.08
	$\xrightarrow{E1} 4p\ ^2P_{3/2}$	-2.083	-2.068	4.28
	$\xrightarrow{M1} 4d\ ^2D_{3/2}$	~ 0	~ 0	~ 0
	$\xrightarrow{E2} 4d\ ^2D_{3/2}$	-26.953	-25.156	632.82
	$\xrightarrow{E2} 4d\ ^2D_{5/2}$	33.052	30.872	953.08
$5p\ ^2P_{1/2}$	$\xrightarrow{E1} 3d\ ^2D_{3/2}$	0.291	0.251	0.06
	$\xrightarrow{E1} 4s\ ^2S_{1/2}$	-0.106	-0.179	0.03
	$\xrightarrow{M1} 4p\ ^2P_{1/2}$	~ 0	~ 0	~ 0
	$\xrightarrow{M1} 4p\ ^2P_{3/2}$	-0.005	-0.005	~ 0

Continue ...

TABLE II – continuation from the previous table.

Transition $i \to f$		Dirac-Fock	CCSD(T)	$S_{i \to f}$
	$\xrightarrow{E2} 4p\ ^2P_{3/2}$	-7.734	-7.403	54.80
	$\xrightarrow{E1} 4d\ ^2D_{3/2}$	4.578	4.330	18.75
	$\xrightarrow{E1} 5s\ ^2S_{1/2}$	4.949	4.849	23.51
$5p\ ^2P_{3/2}$	$\xrightarrow{E1} 3d\ ^2D_{3/2}$	-0.130	-0.113	0.02
	$\xrightarrow{E1} 3d\ ^2D_{5/2}$	0.392	0.340	0.12
	$\xrightarrow{E1} 4s\ ^2S_{1/2}$	-0.132	0.236	0.56
	$\xrightarrow{M1} 4p\ ^2P_{1/2}$	0.005	0.005	~ 0
	$\xrightarrow{E2} 4p\ ^2P_{1/2}$	-7.540	-7.209	51.97
	$\xrightarrow{M1} 4p\ ^2P_{3/2}$	~ 0	~ 0	~ 0
	$\xrightarrow{E2} 4p\ ^2P_{3/2}$	-7.660	-7.332	53.76
	$\xrightarrow{E1} 4d\ ^2D_{5/2}$	-6.124	-5.793	33.56
	$\xrightarrow{E1} 4d\ ^2D_{3/2}$	2.037	1.936	3.75
	$\xrightarrow{E1} 5s\ ^2S_{1/2}$	7.063	6.851	46.94
	$\xrightarrow{M1} 5p\ ^2P_{1/2}$	1.154	1.154	1.33
	$\xrightarrow{E2} 5p\ ^2P_{1/2}$	47.408	45.585	2077.99
$4f\ ^2F_{5/2}$	$\xrightarrow{E1} 3d\ ^2D_{3/2}$	-1.402	-1.173	1.38
	$\xrightarrow{E1} 3d\ ^2D_{5/2}$	-0.376	-0.315	0.011
	$\xrightarrow{E2} 4p\ ^2P_{1/2}$	17.580	16.611	275.92
	$\xrightarrow{M1} 4p\ ^2P_{3/2}$	~ 0	~ 0	~ 0
	$\xrightarrow{E2} 4p\ ^2P_{3/2}$	-9.471	-8.953	80.16
	$\xrightarrow{E1} 4d\ ^2D_{3/2}$	-7.965	-7.570	57.30
	$\xrightarrow{E1} 4d\ ^2D_{5/2}$	-2.130	-2.025	4.10
	$\xrightarrow{E2} 5p\ ^2P_{1/2}$	-45.466	-43.894	1926.68
	$\xrightarrow{M1} 5p\ ^2P_{3/2}$	~ 0	~ 0	~ 0
	$\xrightarrow{E2} 5p\ ^2P_{3/2}$	-24.318	-23.480	551.31
$4f\ ^2F_{7/2}$	$\xrightarrow{E1} 3d\ ^2D_{5/2}$	-1.682	-1.411	1.99
	$\xrightarrow{E2} 4p\ ^2P_{3/2}$	23.12	23.20	538.24
	$\xrightarrow{E1} 4d\ ^2D_{5/2}$	-9.526	-9.055	81.99
	$\xrightarrow{E2} 5p\ ^2P_{3/2}$	59.16	59.56	3547.40
	$\xrightarrow{M1} 4f\ ^2F_{5/2}$	1.852	1.852	3.43
	$\xrightarrow{E2} 4f\ ^2F_{5/2}$	18.25	18.250	333.06
$5d\ ^2D_{3/2}$	$\xrightarrow{M1} 3d\ ^2D_{3/2}$	0.0001	0.000	0.0
	$\xrightarrow{E2} 3d\ ^2D_{3/2}$	-0.976	-0.917	0.84
	$\xrightarrow{M1} 3d\ ^2D_{5/2}$	0.0008	0.003	~ 0
	$\xrightarrow{E2} 3d\ ^2D_{5/2}$	-0.640	-0.602	0.36
	$\xrightarrow{M1} 4s\ ^2S_{1/2}$	~ 0	~ 0	~ 0
	$\xrightarrow{E2} 4s\ ^2S_{1/2}$	-1.856	-1.642	2.70
	$\xrightarrow{E1} 4p\ ^2P_{1/2}$	-0.756	-0.613	0.38
	$\xrightarrow{E1} 4p\ ^2P_{3/2}$	0.334	0.270	0.08
	$\xrightarrow{M1} 4d\ ^2D_{3/2}$	~ 0	-0.001	~ 0
	$\xrightarrow{E2} 4d\ ^2D_{3/2}$	15.562	14.746	217.44
	$\xrightarrow{M1} 4d\ ^2D_{5/2}$	0.001	0.003	~ 0
	$\xrightarrow{E2} 4d\ ^2D_{5/2}$	10.217	9.690	93.90
	$\xrightarrow{M1} 5s\ ^2S_{1/2}$	~ 0	~ 0	~ 0
	$\xrightarrow{E2} 5s\ ^2S_{1/2}$	-31.762	-31.420	987.22
	$\xrightarrow{E1} 5p\ ^2P_{1/2}$	-6.773	-6.731	45.31

Continue ...

TABLE II – continuation from the previous table.

Transition $i \rightarrow f$	Dirac-Fock	CCSD(T)	$S_{i \rightarrow f}$
$\xrightarrow{E1} 5p\ ^2P_{3/2}$	−3.048	−3.030	9.19
$\xrightarrow{E1} 4f\ ^2F_{5/2}$	−5.348	−5.500	30.25
$5d\ ^2D_{5/2} \xrightarrow{M1} 3d\ ^2D_{3/2}$	−0.0007	0.002	~ 0
$\xrightarrow{E2} 3d\ ^2D_{3/2}$	0.638	0.560	0.31
$\xrightarrow{M1} 3d\ ^2D_{5/2}$	0.0003	0.0060	~ 0
$\xrightarrow{E2} 3d\ ^2D_{5/2}$	−1.280	−1.203	1.45
$\xrightarrow{E2} 4s\ ^2S_{1/2}$	−2.280	−2.010	4.04
$\xrightarrow{E1} 4p\ ^2P_{3/2}$	1.006	0.813	0.66
$\xrightarrow{M1} 4d\ ^2D_{3/2}$	0.001	0.0003	~ 0
$\xrightarrow{E2} 4d\ ^2D_{3/2}$	−10.168	−9.635	92.83
$\xrightarrow{M1} 4d\ ^2D_{5/2}$	−0.0002	−0.0060	~ 0
$\xrightarrow{E2} 4d\ ^2D_{5/2}$	20.396	19.344	374.19
$\xrightarrow{E2} 5s\ ^2S_{1/2}$	−38.858	−38.441	1477.71
$\xrightarrow{E1} 5p\ ^2P_{3/2}$	−9.138	−9.082	82.48
$\xrightarrow{E1} 4f\ ^2F_{5/2}$	1.427	1.468	2.16
$\xrightarrow{E1} 4f\ ^2F_{7/2}$	−6.382	−6.564	43.09
$\xrightarrow{M1} 5d\ ^2D_{3/2}$	1.549	1.549	2.40
$\xrightarrow{E2} 5d\ ^2D_{3/2}$	53.712	50.516	2551.87
$6s\ ^2S_{1/2} \xrightarrow{M1} 3d\ ^2D_{3/2}$	~ 0	~ 0	~ 0
$\xrightarrow{E2} 3d\ ^2D_{3/2}$	0.237	0.193	0.04
$\xrightarrow{E2} 3d\ ^2D_{5/2}$	−0.292	−0.240	0.06
$\xrightarrow{M1} 4s\ ^2S_{1/2}$	~ 0	0.002	~ 0
$\xrightarrow{E1} 4p\ ^2P_{1/2}$	0.420	0.428	0.18
$\xrightarrow{E1} 4p\ ^2P_{3/2}$	0.598	0.614	0.38
$\xrightarrow{M1} 4d\ ^2D_{3/2}$	~ 0	~ 0	~ 0
$\xrightarrow{E2} 4d\ ^2D_{3/2}$	−7.347	−6.385	40.77
$\xrightarrow{E2} 4d\ ^2D_{5/2}$	9.039	7.871	61.95
$\xrightarrow{M1} 5s\ ^2S_{1/2}$	~ 0	0.001	~ 0
$\xrightarrow{E1} 5p\ ^2P_{1/2}$	2.922	2.862	8.19
$\xrightarrow{E1} 5p\ ^2P_{3/2}$	−4.182	−4.100	16.81
$\xrightarrow{M1} 5d\ ^2D_{3/2}$	~ 0	~ 0	~ 0
$\xrightarrow{E2} 5d\ ^2D_{3/2}$	86.375	81.81	6692.88
$\xrightarrow{E2} 5d\ ^2D_{5/2}$	−105.891	−100.318	10063.70
$6p\ ^2P_{1/2} \xrightarrow{E1} 3d\ ^2D_{3/2}$	−0.152	−0.128	0.02
$\xrightarrow{E1} 4s\ ^2S_{1/2}$	0.068	0.115	0.01
$\xrightarrow{M1} 4p\ ^2P_{1/2}$	~ 0	~ 0	~ 0
$\xrightarrow{M1} 4p\ ^2P_{3/2}$	0.002	0.003	~ 0
$\xrightarrow{E2} 4p\ ^2P_{3/2}$	2.118	2.074	4.30
$\xrightarrow{E1} 4d\ ^2D_{3/2}$	0.498	0.512	0.26
$\xrightarrow{E1} 5s\ ^2S_{1/2}$	0.054	0.093	0.01
$\xrightarrow{M1} 5p\ ^2P_{1/2}$	~ 0	~ 0	~ 0
$\xrightarrow{M1} 5p\ ^2P_{3/2}$	−0.005	−0.005	~ 0
$\xrightarrow{E2} 5p\ ^2P_{3/2}$	−24.547	−23.634	558.57
$\xrightarrow{E2} 4f\ ^2F_{5/2}$	−18.899	−18.629	347.04
$\xrightarrow{E1} 5d\ ^2D_{3/2}$	8.600	8.168	66.72
$\xrightarrow{E1} 6s\ ^2S_{1/2}$	8.268	8.160	66.58

Continue ...

TABLE II – continuation from the previous table.

Transition $i \rightarrow f$	Dirac-Fock	CCSD(T)	$S_{i \rightarrow f}$
$6p\ ^2P_{3/2} \xrightarrow{E1} 3d\ ^2D_{3/2}$	−0.068	−0.057	0.003
$\xrightarrow{E1} 3d\ ^2D_{5/2}$	0.205	0.174	0.03
$\xrightarrow{E1} 4s\ ^2S_{1/2}$	−0.088	−0.155	0.02
$\xrightarrow{M1} 4p\ ^2P_{1/2}$	0.002	0.002	~ 0
$\xrightarrow{E2} 4p\ ^2P_{1/2}$	−2.092	−2.048	4.19
$\xrightarrow{M1} 4p\ ^2P_{3/2}$	~ 0	~ 0	~ 0
$\xrightarrow{E2} 4p\ ^2P_{3/2}$	2.110	2.068	4.28
$\xrightarrow{E1} 4d\ ^2D_{3/2}$	0.226	0.232	0.05
$\xrightarrow{E1} 4d\ ^2D_{5/2}$	−0.678	−0.696	0.48
$\xrightarrow{E1} 5s\ ^2S_{1/2}$	−0.048	−0.102	0.01
$\xrightarrow{M1} 5p\ ^2P_{1/2}$	0.005	0.005	~ 0
$\xrightarrow{E2} 5p\ ^2P_{1/2}$	−23.928	−22.998	528.90
$\xrightarrow{M1} 5p\ ^2P_{3/2}$	~ 0	0.003	~ 0
$\xrightarrow{E2} 5p\ ^2P_{3/2}$	24.295	23.368	546.06
$\xrightarrow{M1} 4f\ ^2F_{5/2}$	~ 0	~ 0	~ 0
$\xrightarrow{E2} 4f\ ^2F_{5/2}$	−9.998	−9.852	97.06
$\xrightarrow{E2} 4f\ ^2F_{7/2}$	24.489	24.131	582.26
$\xrightarrow{E1} 5d\ ^2D_{3/2}$	3.830	3.636	13.22
$\xrightarrow{E1} 5d\ ^2D_{5/2}$	−11.506	−10.928	119.42
$\xrightarrow{E1} 6s\ ^2S_{1/2}$	−11.676	−11.522	132.76
$\xrightarrow{M1} 6p\ ^2P_{1/2}$	−1.154	−1.154	1.33
$\xrightarrow{E2} 6p\ ^2P_{1/2}$	−133.050	−129.491	16641.00

Using the transition amplitudes/strengths from the CCSD(T) calculations given in Table II and experimental wavelengths estimated from the NIST database energies (given in Table I), we determine the transition rates, emission oscillator strengths and branching ratios of various transitions and present them in Table III. We have also compared our results with other available results for these properties. There are also few calculations available on the transition probabilities and oscillator strengths earlier. Transition probabilities reported by us in our earlier work [16] which were obtained using the same method of the present work, however considering a larger size of configuration interaction space with the availability of a bigger computational resource in order to verify the consistent of the results with respect to our previous calculations. We find the results are still consistent with our previous calculations. Ali and Kim have also calculated these forbidden transition rates [15] using the multi-configuration Dirac-Fock (MCDF) method, their results are also in agreement with us except for the M1 amplitude of the $4s\ ^2S_{1/2} \rightarrow 3d\ ^2D_{3/2}$ transition. In fact the MCDF method is incompetent to account the correlation effects as comprehensively as the RCC method, especially the core-polarization correlations. From our calculations we observe that the above M1 amplitude is about 5.12×10^{-6} at the DF level and the

core-polarization effects through the core correlations aggrandize it to be -0.001 (a.u.) in the CCSD(T) method. This is the main reason for the discrepancy between the results obtained from these two methods and it advocates for the essence of studying the transition properties using a method like our RCC approach. In another work, Zeippen has also employed the SUPERSTRUCTURE program to estimate these forbidden transition rates besides for some other ions by scaling the wave functions and energies. In that work the results are also compared with the above results of Ali and Kim except for the above discussed M1 transition amplitude which is not reported at all. Our results also agree reasonably well with their calculations. In 1975, Wiese and Fuhr have tabulated most of the transition rates and oscillator strengths due to the allowed transitions accumulating from various works [20]. The calculated results reported in their list were obtained from the non-relativistic mean-field methods and other results were taken from the observations.

Most of our results are comparable with the tabulated results, however the present calculations are believed to be meticulous than those are tabulated in the above reference. This may be perceptible while one scrutinizes the discussions in the next paragraph. Along with the results discussed above, we also present the forbidden transition properties for all these transitions although their contributions seem to be irrelevant for the determination of the lifetimes of the excited states those are considered except for the first two (it will be evident later). However, these results could be useful for some other purposes like estimating the higher multipole polarizabilities, Stark shifts etc. Also, the transition properties for the $6s$ and $6p$ states were not known earlier. We also give the branching ratios of all the transitions in the same table when their values are significant up to three decimal places. It is possible by us to estimate these values due to determination all the important transition rates in this work.

TABLE III: Wavelengths (λ in Å), transition rates (A in s^{-1}), oscillator strengths (f) and branching ratios (Γ) from different works. Numbers given as $[k]$ implies $\times 10^k$.

Upper state (f)	Lower state (i)	$\lambda_{f \to i}$	$A^O_{f \to i}$		f		Γ
			Others	Present	Others	Present	Present
$3d_{5/2}$	$\xrightarrow{M1} 3d_{3/2}$	505970.4	$8.32[-5]^a$ $8.32[-5]^b$ $8.24[-5]^c$	$8.33[-5]$		~ 0	~ 1.0
	$\xrightarrow{E2} 3d_{3/2}$		$1.75[-11]^b$ $1.53[-11]^c$	$1.53[-11]$		~ 0	~ 0.0
$4s_{1/2}$	$\xrightarrow{M1} 3d_{3/2}$	3915.53	$1.05[-8]^b$ $1.79[-4]^c$	$1.95[-4]$		~ 0	~ 0.0
	$\xrightarrow{E2} 3d_{3/2}$		7.95^a 8.21^b 7.86^c	7.83		~ 0	0.407
	$\xrightarrow{E2} 3d_{5/2}$	3946.07	11.5^a 11.9^b 11.41^c	11.40		~ 0	0.593
$4p_{1/2}$	$\xrightarrow{E1} 3d_{3/2}$	1610.194	$4.4[8]^d$	$4.26[8]$	0.085^d	0.083	0.389
	$\xrightarrow{E1} 4s_{1/2}$	2734.857	$3.3[8]^d$	$2.72[8]$	0.37^d	0.305	0.610
$4p_{3/2}$	$\xrightarrow{E1} 3d_{3/2}$	1598.00	$4.6[7]^d$	$4.31[7]$	0.018^d	0.017	0.060
	$\xrightarrow{E1} 3d_{5/2}$	1603.06	$4.1[8]^d$	$3.90[8]$	0.10^d	0.100	0.544
	$\xrightarrow{E1} 4s_{1/2}$	2699.87	$3.3[8]^d$	$2.83[8]$	0.73^d	0.618	0.395
	$\xrightarrow{M1} 4p_{1/2}$	211023.9		$9.56[-4]$		~ 0	~ 0.0
	$\xrightarrow{E2} 4p_{1/2}$			$9.18[-8]$		~ 0	~ 0.0
$4d_{3/2}$	$\xrightarrow{M1} 3d_{3/2}$	890.81		$7.95[-4]$		~ 0	~ 0.0
	$\xrightarrow{E2} 3d_{3/2}$			$3.23[3]$		~ 0	~ 0.0
	$\xrightarrow{M1} 3d_{5/2}$	892.38		0.366		~ 0	~ 0.0
	$\xrightarrow{E2} 3d_{5/2}$			$1.39[3]$		~ 0	~ 0.0
	$\xrightarrow{M1} 4s_{1/2}$	1153.16		$2.80[-4]$		~ 0	~ 0.0
	$\xrightarrow{E2} 4s_{1/2}$			$1.29[4]$		~ 0	~ 0.0
	$\xrightarrow{E1} 4p_{1/2}$	1993.89	$9.6[8]^d$	$8.81[8]$	1.1^d	1.050	0.825
	$\xrightarrow{E1} 4p_{3/2}$	2012.91	$1.9[8]^d$	$1.74[8]$	0.11^d	0.106	0.175

Continue ...

TABLE III – continued from previous page.

Upper state (f)	Lower state (i)	$\lambda_{f\to i}$	$A^O_{f\to i}$ Others	Present	f Others	Present	Γ Present
$4d_{5/2}$	$\xrightarrow{M1} 3d_{3/2}$	890.45		0.003		~ 0	~ 0.0
	$\xrightarrow{E2} 3d_{3/2}$			921.285		~ 0	~ 0.0
	$\xrightarrow{M1} 3d_{5/2}$	892.02		0.531		~ 0	~ 0.0
	$\xrightarrow{E2} 3d_{5/2}$			3.71[3]		~ 0	~ 0.0
	$\xrightarrow{E2} 4s_{1/2}$	1152.56		1.30[4]		~ 0	~ 0.0
	$\xrightarrow{E1} 4p_{3/2}$	2011.07	$1.1[9]^d$	1.05[9]	1.0^d	0.955	~ 1.0
	$\xrightarrow{M1} 4d_{3/2}$	2206044.0		1.00[-6]		~ 0	~ 0.0
	$\xrightarrow{E2} 4d_{3/2}$			8.00[-13]		~ 0	~ 0.0
$5s_{1/2}$	$\xrightarrow{M1} 3d_{3/2}$	870.61		2.87[-3]		~ 0	~ 0.0
	$\xrightarrow{E2} 3d_{3/2}$			296.429		~ 0	~ 0.0
	$\xrightarrow{E2} 3d_{5/2}$	872.11		458.998		~ 0	~ 0.0
	$\xrightarrow{M1} 4s_{1/2}$	1119.53		5.54[-2]		~ 0	~ 0.0
	$\xrightarrow{E1} 4p_{1/2}$	1895.44	$2.8[8]^d$	3.12[8]	0.15^d	0.168	0.350
	$\xrightarrow{E1} 4p_{3/2}$	1912.62	$5.4[8]^d$	5.88[8]	0.15^d	0.161	0.653
	$\xrightarrow{M1} 4d_{3/2}$	38389.78		3.43[-9]		~ 0	~ 0.0
	$\xrightarrow{E2} 4d_{3/2}$			4.25[-3]		~ 0	~ 0.0
	$\xrightarrow{E2} 4d_{5/2}$	39069.67		5.86[-3]		~ 0	~ 0.0
$5p_{1/2}$	$\xrightarrow{E1} 3d_{3/2}$	780.60	$1.5[8]^d$	1.35[8]	0.0066^d	0.006	0.448
	$\xrightarrow{E1} 4s_{1/2}$	974.97		3.51[7]		0.005	0.116
	$\xrightarrow{M1} 4p_{1/2}$	1515.09		~ 0		~ 0	~ 0
	$\xrightarrow{M1} 4p_{3/2}$	1526.04		0.113		~ 0	~ 0
	$\xrightarrow{E2} 4p_{3/2}$			3.71[3]		~ 0	~ 0
	$\xrightarrow{E1} 4d_{3/2}$	6309.35	$7.0[7]^d$	7.56[7]	0.21^d	0.226	0.251
	$\xrightarrow{E1} 5s_{1/2}$	7550.22	$5.4[7]^d$	5.53[7]	0.47^d	0.473	0.184
$5p_{3/2}$	$\xrightarrow{E1} 3d_{3/2}$	779.53	$1.5[7]^d$	1.38[7]	0.0014^d	0.001	0.046
	$\xrightarrow{E1} 3d_{5/2}$	780.73	$1.3[8]^d$	1.23[8]	0.0079^d	0.007	0.407
	$\xrightarrow{E1} 4s_{1/2}$	973.29		3.07[7]		0.009	0.101
	$\xrightarrow{M1} 4p_{1/2}$	1511.06		0.005		~ 0	~ 0.0
	$\xrightarrow{E2} 4p_{1/2}$			1.85[3]		~ 0	~ 0.0
	$\xrightarrow{M1} 4p_{3/2}$	1521.95		5.92[-5]		~ 0	~ 0.0
	$\xrightarrow{E2} 4p_{3/2}$			1.84[3]		~ 0	~ 0.0
	$\xrightarrow{E1} 4d_{3/2}$	6240.04	$7.72[6]^d$	7.74[6]	0.042^d	0.045	0.026
	$\xrightarrow{E1} 4d_{5/2}$	6257.74	$6.5[7]^d$	6.94[7]	0.25^d	0.272	0.229
	$\xrightarrow{E1} 5s_{1/2}$	7451.19	$5.7[7]^d$	5.75[7]	0.94^d	0.957	0.190
	$\xrightarrow{M1} 5p_{1/2}$	568085.0		4.90[-5]		~ 0	~ 0
	$\xrightarrow{E2} 5p_{1/2}$			9.83[-9]		~ 0	~ 0
	$\xrightarrow{M1} 5p_{1/2}$	1521.96		5.92[-5]		~ 0	~ 0
	$\xrightarrow{E2} 5p_{1/2}$			1.84[3]		~ 0	~ 0
$4f_{5/2}$	$\xrightarrow{E1} 3d_{3/2}$	730.60	$1.1[9]^d$	1.19[9]	0.13^d	0.143	0.751
	$\xrightarrow{E1} 3d_{5/2}$	731.66	$7.8[7]^d$	8.59[7]	0.0062^d	0.007	0.051
	$\xrightarrow{E2} 4p_{1/2}$	337.443		1.20[4]		~ 0	~ 0
	$\xrightarrow{M1} 4p_{3/2}$	1345.97		2.56[-6]		~ 0	~ 0
	$\xrightarrow{E2} 4p_{3/2}$			3.39[3]		~ 0	~ 0
	$\xrightarrow{E1} 4d_{3/2}$	4062.36	$2.9[8]^d$	2.89[8]	1.1^d	1.072	0.182
	$\xrightarrow{E1} 4d_{5/2}$	4069.85	$2.1[7]^d$	2.05[7]	0.052^d	0.051	0.013
	$\xrightarrow{E2} 5p_{1/2}$	11406.74		1.862		~ 0	~ 0

Continue ...

TABLE III – continued from previous page.

Upper state (f)	Lower state (i)	$\lambda_{f\to i}$	$A^{\mathrm{O}}_{f\to i}$ Others	Present	f Others	Present	Γ Present
	$\xrightarrow{M1} 5p_{3/2}$	11640.47		1.35[-11]		~ 0	~ 0
	$\xrightarrow{E2} 5p_{3/2}$			0.481		~ 0	~ 0
$4f_{7/2}$	$\xrightarrow{E1} 3d_{5/2}$	731.65	$1.1[9]^d$	1.29[9]	0.12^d	0.138	0.807
	$\xrightarrow{E2} 4p_{3/2}$	1345.97		1.71[4]		~ 0	~ 0
	$\xrightarrow{E1} 4d_{5/2}$	4069.81	$3.1[8]^d$	3.08[8]	1.0^d	1.021	0.192
	$\xrightarrow{E2} 5p_{3/2}$	11640.13		2.323		~ 0	~ 0
	$\xrightarrow{M1} 4f_{5/2}$	4.00[8]		1.81[-13]		~ 0	~ 0
	$\xrightarrow{E2} 4f_{5/2}$			4.55[-24]		~ 0	~ 0
$5d_{3/2}$	$\xrightarrow{M1} 3d_{3/2}$	676.58		3.46[-3]		~ 0	~ 0
	$\xrightarrow{E2} 3d_{3/2}$			1.66[3]		~ 0	~ 0
	$\xrightarrow{M1} 3d_{5/2}$	1954.32		0.001		~ 0	~ 0
	$\xrightarrow{E2} 3d_{5/2}$	677.74		710.019		~ 0	~ 0
	$\xrightarrow{M1} 4s_{1/2}$	827.02		2.93[-4]		~ 0	~ 0
	$\xrightarrow{E2} 4s_{1/2}$			1.95[3]		~ 0	~ 0
	$\xrightarrow{E1} 4p_{1/2}$	1159.22	$1.6[8]^d$	1.22[8]	0.067^d	0.050	0.312
	$\xrightarrow{E1} 4p_{3/2}$	1179.62	$3.2[7]^d$	2.25[7]	0.0066^d	0.005	0.057
	$\xrightarrow{M1} 4d_{3/2}$	2775.75	~ 0		~ 0	~ 0	
	$\xrightarrow{E2} 4d_{3/2}$			369.313		~ 0	~ 0
	$\xrightarrow{M1} 4d_{5/2}$	2783.66		2.09[-4]		~ 0	~ 0
	$\xrightarrow{E2} 4d_{5/2}$	2783.67		157.227		~ 0	~ 0
	$\xrightarrow{M1} 5s_{1/2}$	2996.10		9.03[-7]		~ 0	~ 0
	$\xrightarrow{E2} 5s_{1/2}$			1.14[3]		~ 0	~ 0
	$\xrightarrow{E1} 5p_{1/2}$	4971.28	$1.8[8]^d$	1.87[8]	1.4^d	1.386	0.479
	$\xrightarrow{E1} 5p_{3/2}$	5016.73	$3.6[7]^d$	3.68[7]	0.14^d	0.139	0.094
	$\xrightarrow{E1} 4f_{5/2}$	8817.62	$2.1[7]^d$	2.23[7]	0.16^d	0.173	0.057
$5d_{5/2}$	$\xrightarrow{M1} 3d_{3/2}$	674.99		0.004		~ 0	~ 0
	$\xrightarrow{E2} 3d_{3/2}$			479.243		~ 0	~ 0
	$\xrightarrow{M1} 3d_{5/2}$	675.89		0.494		~ 0	~ 0
	$\xrightarrow{E2} 3d_{5/2}$			2.2[3]		~ 0	~ 0
	$\xrightarrow{E2} 4s_{1/2}$	815.59		2.11[3]		~ 0	~ 0
	$\xrightarrow{E1} 4p_{3/2}$	1168.61	$1.9[8]^d$	1.40[8]	0.060^d	0.043	0.368
	$\xrightarrow{M1} 4d_{3/2}$	2786.09		1.50[-5]		~ 0	~ 0
	$\xrightarrow{E2} 4d_{3/2}$			103.186		~ 0	~ 0
	$\xrightarrow{M1} 4d_{5/2}$	2789.62		6.55[-3]		~ 0	~ 0
	$\xrightarrow{E2} 4d_{5/2}$			413.268		~ 0	~ 0
	$\xrightarrow{E2} 5s_{1/2}$	3004.12		1.13[3]		~ 0	~ 0
	$\xrightarrow{E1} 5p_{3/2}$	5033.47	$2.2[8]^d$	2.18[8]	1.2^d	1.242	0.573
	$\xrightarrow{E1} 4f_{5/2}$	8868.18	$0.99[6]^d$	1.04[6]	0.012^d	0.012	0.023
	$\xrightarrow{E1} 4f_{7/2}$	8868.38	$2.0[7]^d$	2.09[7]	0.18^d	0.185	0.055
	$\xrightarrow{M1} 5d_{3/2}$	4972650.0		8.78[-8]		~ 0	~ 0
	$\xrightarrow{E2} 5d_{3/2}$			1.57[-13]		~ 0	~ 0
$6s_{1/2}$	$\xrightarrow{M1} 3d_{3/2}$	670.27		2.07[-3]		~ 0	~ 0
	$\xrightarrow{E2} 3d_{3/2}$			1.54[2]		~ 0	~ 0
	$\xrightarrow{E2} 3d_{5/2}$	671.16		237.108		~ 0	~ 0
	$\xrightarrow{M1} 4s_{1/2}$	808.70		6.53[-2]		~ 0	~ 0
	$\xrightarrow{E1} 4p_{1/2}$	1148.24		1.23[8]		0.024	0.201

Continue . . .

TABLE III – continued from previous page.

Upper state (f)	Lower state (i)	$\lambda_{f\to i}$	$A^{\mathrm{O}}_{f\to i}$ Others	Present	f Others	Present	Γ Present
	$\xrightarrow{E1} 4p_{3/2}$	1154.52		2.48[8]		0.025	0.406
	$\xrightarrow{M1} 4d_{3/2}$	2707.36		6.80[-6]		~ 0	~ 0
	$\xrightarrow{E2} 4d_{3/2}$			156.908		~ 0	~ 0
	$\xrightarrow{E2} 4d_{5/2}$	2710.68		236.973		~ 0	~ 0
	$\xrightarrow{M1} 5s_{1/2}$	2912.77		5.46[-4]		~ 0	~ 0
	$\xrightarrow{E1} 5p_{1/2}$	4742.28		7.78[7]		0.262	0.127
	$\xrightarrow{E1} 5p_{3/2}$	4782.20		1.62[8]		0.278	0.265
	$\xrightarrow{M1} 5d_{3/2}$	93984.96		3.09[-11]		~ 0	~ 0
	$\xrightarrow{E2} 5d_{3/2}$			5.11[-4]		~ 0	~ 0
	$\xrightarrow{E2} 5d_{5/2}$	95795.53		6.98[-4]		~ 0	~ 0
$6p_{1/2}$	$\xrightarrow{E1} 3d_{3/2}$	643.13		6.27[7]		0.002	0.397
	$\xrightarrow{E1} 4s_{1/2}$	769.52		2.96[7]		0.003	0.187
	$\xrightarrow{M1} 4p_{1/2}$	1070.83		4.40[-4]		~ 0	~ 0
	$\xrightarrow{M1} 4p_{3/2}$	1076.29		0.009		~ 0	~ 0
	$\xrightarrow{E2} 4p_{3/2}$			1.67[3]		~ 0	~ 0
	$\xrightarrow{E1} 4d_{3/2}$	2313.09		2.15[7]		0.009	0.136
	$\xrightarrow{E1} 5s_{1/2}$	2461.40		5.99[5]		0.0005	0.004
	$\xrightarrow{M1} 5p_{1/2}$	3651.94		4.43[-5]		~ 0	~ 0
	$\xrightarrow{M1} 5p_{3/2}$	3675.58		6.04[-3]		~ 0	~ 0
	$\xrightarrow{E2} 5p_{3/2}$	3675.58		465.653		~ 0	~ 0
	$\xrightarrow{E2} 4f_{5/2}$	5371.75		43.43		~ 0	~ 0
	$\xrightarrow{E1} 5d_{3/2}$	13587.42		2.69[7]		0.372	0.170
	$\xrightarrow{E1} 6s_{1/2}$	15883.73		1.68[7]		0.635	0.106
$6p_{3/2}$	$\xrightarrow{E1} 3d_{3/2}$	642.78		6.41[6]		0.0004	0.040
	$\xrightarrow{E1} 3d_{5/2}$	643.59		5.75[7]		0.002	0.363
	$\xrightarrow{E1} 4s_{1/2}$	769.02		2.68[7]		0.005	0.169
	$\xrightarrow{M1} 4p_{1/2}$	1069.85		0.003		~ 0	~ 0
	$\xrightarrow{E2} 4p_{1/2}$			837.868		~ 0	~ 0
	$\xrightarrow{M1} 4p_{3/2}$	1075.3		0.010		~ 0	~ 0
	$\xrightarrow{E2} 4p_{3/2}$			1.32[3]		~ 0	~ 0
	$\xrightarrow{E1} 4d_{3/2}$	2308.53		2.22[6]		0.002	0.014
	$\xrightarrow{E1} 4d_{5/2}$	2310.95		1.99[7]		0.011	0.126
	$\xrightarrow{E1} 5s_{1/2}$	2456.24		3.55[5]		0.0006	0.002
	$\xrightarrow{M1} 5p_{1/2}$	3640.59		4.59[-3]		~ 0	~ 0
	$\xrightarrow{E2} 5p_{1/2}$			231.479		~ 0	~ 0
	$\xrightarrow{M1} 5p_{3/2}$	3664.07		1.23[-3]		~ 0	~ 0
	$\xrightarrow{E2} 5p_{3/2}$			2.31[2]		~ 0	~ 0
	$\xrightarrow{M1} 4f_{5/2}$	5347.21		4.41[-11]		~ 0	~ 0
	$\xrightarrow{E2} 4f_{5/2}$			6.21[1]		~ 0	~ 0
	$\xrightarrow{E2} 4f_{7/2}$	5347.28		3.72[1]		~ 0	~ 0
	$\xrightarrow{E1} 5d_{5/2}$	13467.90		2.48[7]		0.451	0.157
	$\xrightarrow{E1} 5d_{3/2}$	13431.53		2.76[6]		0.075	0.017
	$\xrightarrow{E1} 6s_{1/2}$	15671.11		1.75[7]		1.289	0.110
	$\xrightarrow{M1} 6p_{1/2}$	1170686.0		5.60[-6]		~ 0	~ 0
	$\xrightarrow{E2} 6p_{1/2}$			2.13[-9]		~ 0	~ 0

References: [a] [14]; [b] [15]; [c] [16]; [d] [20].

In comparison to the above transition properties, it is

observed that insufficient efforts are being made to accomplish any reliable results for the lifetimes of different states in Sc III. Andersen et al [13] have measured lifetimes of the $4p$ states. In an outdated work, Buchta et al had carried out investigation of the lifetimes of a number of states in the considered ion using a beam-foil technique measurement with reasonable accuracies [12]. Some of the data reported by Wiese and Fuhr [20], as was mentioned in the previous paragraph, were actually quoted from these measurements. We have estimated the lifetimes of all the states that we have taken into account for our study using the transition rates given above and listed them in Table IV along side the results of Andersen et al and Buchta et al. We have also estimated uncertainties from the neglected Breit interaction and correlation effects (slightly larger values are taken as upper limits) and they are quoted inside the parentheses. Our estimated lifetimes for the $4f$ states are completely disaccord with the results reported in [12]. The cause for the large discrepancies between these results could be due to the anticipated error in the measurement as mentioned by Buchta et al in their paper; instead these measurements may correspond to the lifetimes of the cascade $5g$ states. We have also referred to few other theoretical estimations of the lifetimes of the $4p$ states in the same table which were, in fact, determined from the mean-field theory based calculations. From the agreement between the measured lifetimes for the $4p$ states with the mean-field theory results using the velocity gauge expression than the length gauge expression, Buchta et al have justified the accuracy of the mean-field based calculation and their results [12]. However, this agreement may be accidental, because as we have stated in the earlier paragraph that the transition amplitudes from the DF method (mean-field theory calculation) are usually larger in magnitudes compared to the results obtained from the RCC method. So the mean-field results are expected to give smaller lifetime values and the same was observed in the mean-field theory calculation. It is well known fact that the length gauge expression gives faster converged amplitude result than the velocity gauge expression in an approximated many-body theory calculations. Further, Buchta et al have given other examples like how they find a similar observation for the estimation of the lifetimes of the $4p$ states in the calcium ion (Ca II). We have also studied the lifetimes of various states using the length gauge expression in Ca II using our CCSD(T) method [18, 27] and shown the importance of the correlation effects to obtain results agreeing the with their corresponding measured values. Therefore, we think that the estimated lifetimes of the $4p$ states for Sc III in this work are more precise than the measurements by Buchta et al [12]. It would be appropriate to carry out further measurements of the lifetimes of different states in this ion using the the modern advanced experimental techniques to probe their accuracies and test the potential of the many-body methods to reproduce them.

The lifetime and oscillator strength of the $5s$ state and

TABLE IV: Lifetimes (τ) of low-lying states in Sc III.

State	This work	Others	Experiments
		Lifetimes in s	
$3d\ ^2D_{5/2}$	12135(100)	12130.86[a]	
$4s\ ^2S_{1/2}$	0.05(1)	0.0519[a]	
		Lifetimes in ns	
$4p\ ^2P_{1/2}$	1.43(2)	1.6[b]	1.7(2)[b,d]
$4p\ ^2P_{3/2}$	1.40(3)	1.27/1.66[c]	1.7(2)[b,d]
$4d\ ^2D_{3/2}$	0.95(1)		1.2(2)[d]
$4d\ ^2D_{5/2}$	0.96(3)		1.2(2)[d]
$5s\ ^2S_{1/2}$	1.08(2)		1.4(2)[d]
$5p\ ^2P_{1/2}$	3.32(2)		3.6(4)[d]
$5p\ ^2P_{3/2}$	3.31(3)		3.6(4)[d]
$4f\ ^2F_{5/2}$	0.61(1)		3.5(8)[d]
$4f\ ^2F_{7/2}$	0.63(2)		3.5(8)[d]
$5d\ ^2D_{3/2}$	2.56(1)		2.4(3)[d]
$5d\ ^2D_{5/2}$	2.63(1)		2.4(3)[d]
$6s\ ^2S_{1/2}$	1.66(1)		
$6p\ ^2P_{1/2}$	6.32(9)		
$6p\ ^2P_{3/2}$	6.33(8)		

References: [a] [16]; [b] [13]; [c] [26]; [d] [12].

$4p - 5s$ transition in Sc III were reported as $1.4(2)ns$ and $0.13(2)$ in [12], which we obtain as $1.08(2)ns$ and 0.168, respectively. Our oscillator strength for the above transition match well with the tabulated result as 0.15 in [20]. Nonetheless, our results for the $5d$ states agree substantially with the results reported by Buchta et al [12]. The measured oscillator strength for the $3d \to 4f$ transition is reported as 0.03 which differ completely from our result 0.14, but our result agrees with the results reported in [20]. With all the above observations, it is worth reiterating that the results reported in this work are more accurate and they can be used reliably in any other applications.

Using the forbidden transition amplitudes, we find very large lifetimes for the $3d\ ^2D_{5/2}$ and $4s\ ^2S_{1/2}$ states. The lifetime of the $3d\ ^2D_{5/2}$ state is found to be $12135s$ which is very large, because of the highly forbidden transition between the corresponding fine structure states (EE is very small). The lifetime of the $4s\ ^2S_{1/2}$ state found to be $0.05s$ which is also large enough in an atomic scale for carrying out any other precision studies related to this state. These results are also in perfect agreement with our previous findings [16].

IV.   CONCLUSION

We have employed the relativistic coupled-cluster method to determine both the allowed and forbidden

transition amplitudes in the doubly ionized scandium. By combining these results with the experimental wavelengths, we have estimated the transition rates, oscillator strengths, branching ratios and lifetimes for the first sixteen states in this ion. We have compared our results with the previously reported ones and find a reasonably agreement between them. The reported lifetimes of various states in this work seem to be meticulous than the previously available results. Our results can be instrumental for various astrophysical studies embodying scandium element. Further, these results can also be directive for the new experiments to affirm the accuracies of the reported properties.

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