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 correlations due to the Coulomb interaction to all orders by considering all possible singly and doubly excited electronic configurations conjointly with the contributions from the leading order triple excitations in a perturbative approach. Present results are compared with the previously available results for the transition lines of astrophysical interest and the role of the correlation effects are also discussed concisely. Some of the transition rates, oscillator strengths and lifetimes are acquainted.

I. INTRODUCTION

The low-lying energy spectra of the doubly ionized scandium (Sc III) have been measured long time ago [1–3], however accurate results for other transition properties which are of astrophysical interest are almost diminutive. Sc is one of the important elements available in the photosphere of sun [4–7]. With the accurate information of the spectroscopic data of Sc and its ions, one can procure palpable knowledge about the abundance of this element in the solar photosphere [5, 6]. Even after the report on the abundances of different elements in the sun by Anders et al [8], Sc abundance is not yet updated for the solar photosphere. Spectroscopic data of Sc can also serve as reference to determine abundances of other elements in the metal-poor stars [5]. 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 [5, 7]. Ambiguity in the finding of the overabundant of Sc in most of the metal rich stars [9] can be resolved from the improved its 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 [10]. Intensities of these transitions are vital to infer knowledge about the plasma temperature and dynamics which are of crucial quantities in the determination of the electron density and temperature diagnostics for many astronomical objects and in the laboratory tokamak plasmas [10].

Sc III belongs to the potassium (K I) isoelectronic sequence, but their energy level sequences 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 calculations of the transition rates, oscillator strengths and lifetimes for different states in Sc III are available yet and most of them are obtained using the mean-field theories. Many of the theoretical and observed properties of Sc III are given in [11–15], out of which our previous reported results on the transition rates and lifetimes of the 3d and 4s states in this ion [15] are 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 compile with a large 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 punctiliously [16–18]. Some of the data are being tabulated through all the stages of ionization in Sc by Wiese and Fuhr [19] and we make a comparison analysis of Sc III results.

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 channelized transitions. Then we pursue with presenting and discussing the results in the following section before summarizing them.

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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 [20]

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

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 E_k values [20].

In the macroscopic mechanical equilibrium and given the input of the gas density, optical depth of the stellar atmosphere can be reckoned by [21]

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

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 oscillator strengths are also necessary for this purpose.

The emission (absorption) oscillator strength f_{ki} (f_{ik}) is given by [22]

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

where λ_{ki} and the transition probability rate A_{ki} are used in Å and s^{-1}, respectively. Sometime the weighted oscillator strengths are also used which can be deduced 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

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

where we are not accounting contributions from the $M2$ and $E3$ channels due to their negligible transition rates compared to the considered channels. In the above equations, units of A_{ki} and λ_{ki} are maintained with the previous expression, the line strengths are given in atomic unit (a.u.) for the corresponding channel O which is 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

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

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, 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 [16, 23])

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

where T and S_v represent the excitation operators formulated through the core-core and core-valence electron correlation effects, respectively. In this work, we consider all possible single and double excitations to all orders and triple excitations only due to leading orders of perturbation in a self-consistent procedure; commonly known as the (R)CCSD(T) method. Since Sc III is a medium size atomic system, CCSD(T) method can apprehend the correlation effects comprehensively.

Excitation amplitudes for T operators are determined from 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 (negative of the ionization potential (IP)) and S_v amplitudes simultaneously for a given ASF with valence electron v by solving the expression

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

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

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

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

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 [16, 23].

The trial DF wave function $|\Phi_0\rangle$ is constructed initially using the Gaussian type orbitals (GTOs) before obtaining the self-consistent solutions. To obtain RCC wave functions, we have considered interaction space within 15s, 15p, 15d, 13f and 12g orbitals.

III. RESULTS AND DISCUSSIONS

We present first the IP results of various states from this work using DF and CCSD(T) methods and compare them in Table I with the corresponding values given in the NIST database [24]. 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; actually 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 correct results in the considered system.

Although the calculated IP results seem to be accurate enough for considering them in the *ab initio* determination of transition properties, but it can be noticed that the errors associated in the energies get augmented in the estimation of excitation energies (EEs); especially between the fine structure states. This is because of the expected non-negligible contribution from other higher relativistic corrections from QED and Breit interactions which are neglected in the present work. In contrast to the energies, the QED and Breit interaction contributions are accustomed to be very small in the estimation of transition amplitudes. To elude from the large uncertainties, we use the experimental energies to find out the wavelengths of all the considered transitions.

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 polarizabilities of different

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 [24] (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

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 M1 transition amplitudes are also large enough to be accounted for. Role of the correlations to determine these properties can be observed 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 transition 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

Continue ...

TABLE II – continuation from the previous table.

Transition $i \to f$	Dirac-Fock	CCSD(T)	$S_{i \to f}$
$\xrightarrow{E1}$ 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
$\xrightarrow{E2}$ 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
$\xrightarrow{E1}$ 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

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TABLE II – continuation from the previous table.

Transition $i \to f$	Dirac-Fock	CCSD(T)	$S_{i \to f}$
$\xrightarrow{E1} 5p\ ^2P_{3/2}$	-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
$6p\ ^2P_{3/2}$ $\xrightarrow{E1} 3d\ ^2D_{3/2}$	-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

Continue ...

TABLE II – continuation from the previous table.

Transition $i \to f$	Dirac-Fock	CCSD(T)	$S_{i \to f}$
$\xrightarrow{E2} 5p\ ^2P_{3/2}$	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 amplitudes 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 the above properties. There are also few calculations available on the transition probabilities and oscillator strengths earlier. Transition probabilities reported by us in our earlier work [15] which were obtained using the same method of the present work, however we have considered a large configuration interaction space in this work to account for the correlation effects numerously. We find the results are still consistent with our previous findings. Ali and Kim have also calculated these forbidden transition rates [14] using the multi-configuration Dirac-Fock (MCDF) method, their results are also in agreement with us except for the M1 amplitude of the $4s\ ^2S_{1/2} \to 3d\ ^2D_{3/2}$ transition. In fact the MCDF method is incompetent to account 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. Therefore, this is the reason for the discrepancy between the results obtained from two methods and it advocates for the essence of studying the transition properties using a method like our RCC theory. In another work, Zeippen has also employed 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 [19]. The calculated results reported in this 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 following discussions. In addition to these results, we also augment the forbidden transition properties in conjunction with the allowed transitions involving the $6s$ and $6p$ states those

are not studied ever till date. Nevertheless, the branching ratios of all these transitions are also not investigated categorically anywhere due to the lack of substantial information about all the important transitions. In the above table, we present these results after ignoring the insignificant transition rate contributions from the higher multipoles like M2, E3 etc., channels.

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
$4d_{5/2}$	$\xrightarrow{M1} 3d_{3/2}$	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

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
	$\xrightarrow{E2} 3d_{5/2}$	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
	$\xrightarrow{M1} 5p_{3/2}$	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

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
	$\xrightarrow{M1} 3d_{5/2}$ 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
	$\xrightarrow{E1} 4p_{3/2}$ 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

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
$6p_{1/2}$	$\xrightarrow{E1} 3d_{3/2}$	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] [13]; [b] [14]; [c] [15]; [d] [19].

In comparison to the above transition properties, it is observed that imperceptible efforts are made for accomplishing any reliable results for the lifetimes of different states in Sc III. Andersen et al [12] have measured lifetimes of the 4p states. In an antique 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 [11]. Some of the data reported by Wiese and Fuhr [19], as was mentioned in the previous paragraph, were in fact quoted from these measurements. We have estimated the life-times 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 given as upper limits) and they are quoted inside the parentheses. Our lifetime estimations for the 4f states are completely disaccord with the results reported in [11]. The cause for the large discrepancies between these results could be due to the explanation given by Buchta et al in their paper as it may be corresponding to the lifetimes of the cascade 5g

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] [15]; [b] [12]; [c] [25]; [d] [11].

states instead of the $4f$ states. We have also referred to few theoretical estimations of the lifetimes of the $4p$ states in the same table which are, in fact, determined from the mean-field theory based calculations. With that respect, our results seem to be exquisite. As we had emphasized earlier while discussing results from Table II, the transition amplitudes obtained from DF calculations are generally larger in magnitudes compared to the RCC results. So it is nominal to achieve smaller values of lifetimes when DF or mean-field theory based calculations are taken into account depriving the electron correlation effects. Therefore, it deceives the justification of the accuracy of the results reported in [11] by comparing with mean-field results from the velocity gauge expression. It also has to be brought into notice that calculations with velocity gauge expression do not converge faster than the calculations with the length gauge expression with respect to the configuration interaction space. Further, it is contended by Buchta et al in favour of these agreements by referring to a similar comparison of the results for the $4p$ states in the doubly ionized calcium (Ca II). Using our same CCSD(T) method that is considered here, we we have also estimated the lifetimes of different states in Ca II with fair certainties in some of our recent studies [17, 26].

The lifetime and oscillator strength of the $5s$ state and $4p-5s$ transition in Sc III were reported as $1.4(2)ns$ and

0.13(2) in [11] against our results $1.08(2)ns$ and 0.168, respectively. Our oscillator strength for the above transition match well with the tabulated result 0.15 in [19]. Nonetheless, our results for the $5d$ states agree substantially with the results reported by Buchta et al. Again, the oscillator strength for the $3d \to 4f$ transition is reported as 0.03 which digresses completely our result 0.14 which further acquiesces with the results reported in [19]. Capitulating all the above discussions, the results reported from the present work can be presumed to be more scrupulous to be considered for further utilization.

From the forbidden transition studies, we find very large lifetimes for the $3d\ ^2D_{5/2}$ and $4s\ ^2S_{1/2}$ states. The lifetime of the $3d\ ^2D_{5/2}$ is found to be $12135s$ which is very large, almost stable, because of the highly forbidden between the corresponding fine structure transitions (EE is very small). The lifetime of the $4s\ ^2S_{1/2}$ state found to be $0.05s$ which is large enough in an atomic scale for carrying out any precision studies related to this state. These results also agree with our previous findings [15]. Since our reported transition rates related to these transitions are also in good agreement with the previously reported works which are mentioned in Table III, the predicted lifetimes of the above two metastable states seem to be conscientious.

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.

[1] R. C. Gibbs and H. E. White, Proc. Nat. Acad. Sci. US **12**, 598 (1926).

[2] S. Smith, Proc. Nat. Acad. Sci. US **13**, 65 (1927).

[3] J. -E. Holmström, Phys. Scr. **5**, 249 (1972).

[4] K. Lodders, Astrophys. J. **591**, 1220 (2003).

[5] H. W. Zhang, T. Gehren and G. Zhao, *The Art of Modelling Stars in the* 21st *Century*, Proceedings of International Astronomical Union Symposium No. 252, p. 127 (2008).

[6] H. W. Zhang, T. Gehren and G. Zhao, Astron. Astroph. **481**, 489 (2008).

[7] P. Francois, F. Matteucci, R. Cayrel, M. Spite and C. Chiappini, Astron. Astroph. **421**, 613 (2004).

[8] E. Anders and N. Grevesse, Geochim. Cosmochim. Act **53**, 197 (1989).

[9] S. Feltzing and G. Gonzalez, Astron. Astroph. **367**, 253 (2001).

[10] E. Charro, Z. Curiel and I. Martin, Astron. Astroph. **387**, 1146 (2002) and *references therein.*

[11] R. Buchta, L. J. Curtis, I. Martinson and J. Brzozowski, Phys. Scr. **4**, 55 (1971).

[12] T. Andersen, P. Petersen and E. Biemont, J. Quant. Spectrosc. Radiat. Transfer **17**, 389 (1977).

[13] C. Z. Zeippen, Astron. Astroph. **229**, 248 (1990).

[14] M. A. Ali and Y.-Ki Kim, Phys. Rev. A **38**, 3992 (1988).

[15] B. K. Sahoo, H. S. Nataraj, B. P. Das, R. K. Chaudhuri and D. Mukherjee, J. Phys. B **41**, 055702 (2008).

[16] B. K. Sahoo, S. Majumder, R. K. Chaudhuri, B. P. Das and D. Mukherjee, J. Phys. B **37**, 3409 (2004).

[17] B. K. Sahoo, Md. R. Islam, B. P. Das, R. K. Chaudhuri and Debashis Mukherjee, Phys. Rev. A **74**, 062504 (2006).

[18] B. K. Sahoo and B. P. Das, Phys. Rev. A **84**, 012501 (2011).

[19] W. L. Wiese and J. R. Fuhr, J. Phys. Chem. Ref. Data **4**, 263 (1975).

[20] A. Goly, Astron. Astroph. **68**, 79 (1978).

[21] M. S. Dimitrijevic, Mem. S. A. It. Suppl. **15**, 32 (2010).

[22] I. I. Sobelman, *Atomic Spectra and Radiative Transitions*, Springer-Verlag (Berlin), pp. 223 (1979).

[23] D. Mukherjee, B. K. Sahoo, H. S. Nataraj and B. P. Das, J. Phys. Chem. A **113**, 12549 (2009).

[24] http://physics.nist.gov/cgi-bin/ASD/energy1.pl

[25] A. W. Weiss, J. Research Nat. Bur. Standards **71A**, 157 (1967).

[26] B. K. Sahoo, B. P. Das and D. Mukherjee, Phys. Rev. A **79**, 052511 (2009).