Sc III spectral properties of astrophysical interest

D K Nandy1, Y Singh1, B K Sahoo1 and C Li2

1 Theoretical Physics Division, Physical Research Laboratory, Ahmedabad 380009, India
2 State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, People’s Republic of China

E-mail: bijaya@prl.res.in

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Abstract

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 a few low-lying states are given for the first time. The role of the correlation effects in the evaluation of the transition strengths are described concisely.

1. 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 distinct knowledge about the abundance of this element in the solar photosphere [6, 7]. Abundances of different elements in the sun were studied latest by Anders et al [9], but the Sc abundance is not known well 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 a 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 overabundance 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-exitations of the metastable states are rather slow which can lead to the build-up of populations 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 in the determination of the electron densities and temperature diagnostics in many astronomical objects and in the laboratory tokamak plasmas [11]. These data are also of great interest to the experimentalists and theorists for accurate analysis of the scattering processes [1, 12].

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 a 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 the transition rates, oscillator strengths and lifetimes for a number of states in Sc III are available to date and most of them are just using the mean-field theories. These results are studied in different contexts in [13–18]. Our previous reported results [18] were on the transition rates and lifetimes of the 3d and 4s states in this ion. We had evaluated these quantities by calculating the forbidden transition amplitudes using the single-reference open-shell Fock space relativistic coupled-cluster (RCC) method, an all-order perturbative many-body approach (e.g. see [18–20]).
In this 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. We have also studied these properties very accurately using the same employed method in other systems [21–23]. Some of the Sc data through all stages of ionization were being tabulated by Wiese and Fuhr [24] a few decades ago and the corresponding Sc III data can be replaced by the results obtained from the present study for their use in other applications, especially in astrophysical studies.

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 summarizing them.

2. 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 [25]

\[
I_{ki} = \frac{2 \pi \hbar c^2}{m_e} \frac{g_i f_{ik} n}{\lambda_{ki}^3} \exp(-E_k/k_B T),
\]

(2.1)

where \( \lambda_{ki}, f_{ik}, g_i, E_k, n, u \) 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, \( \hbar, c, m_e \) 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 with the reported results to demonstrate the potency of the employed method. Moreover, the temperature of an astrophysical object can be determined by plotting \( \ln I_{ki} \) against the \( E_k \) values [25].

In the macroscopic mechanical equilibrium and with the knowledge of the gas density, the optical depth of the stellar atmosphere can be found by [26]

\[
\tau_{ki} = \int_0^\infty d^3 r \frac{\pi e^2}{m_e c} f_{ik} \rho_i ,
\]

(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 \( \rho_i \) 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 [27]

\[
f_{ki} = 1.4992 \times 10^{-16} A_{ki} \frac{g_k}{g_i} \lambda_{ki}^2 ,
\]

(2.3)

where \( \lambda_{ki} \) and the transition rate \( A_{ki} \) are used in Å and s\(^{-1}\), respectively. Sometimes it is useful to give these quantities in terms of the weighted oscillator strengths (\( f_w \)) which are independent of the emission or absorption lines and defined as

\[
f_w = g_k f_{ki} = -g_i f_{ik} ,
\]

(2.4)

with \( g_i = (2J_i + 1) \) for \( J_i \), being the angular momentum of the state \( |i\rangle \).

The transition rates due to E1, E2 and M1 channels are given by

\[
A_{ki}^{E1} = \frac{2.026 \times 10^{18}}{\lambda_{ki}^3} \delta_{ki} ,
\]

(2.5)

\[
A_{ki}^{E2} = \frac{1.11995 \times 10^{18}}{\lambda_{ki}^5} \delta_{ki} ,
\]

(2.6)

and

\[
A_{ki}^{M1} = \frac{2.69735 \times 10^{13}}{\lambda_{ki}^3} \delta_{ki} ,
\]

(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 \( \lambda_{ki} \) are maintained with equation (2.3) and the line strengths are given in atomic units (au) for the corresponding channel \( O \) which are defined as

\[
S_{ki}^O = \langle \lambda_{ki} \rangle |\langle O|J_i \rangle |^2 .
\]

Now, the single particle expressions for the E1 and E2 multipoles in the length gauge are given by

\[
\langle \kappa_f \mid |\kappa_i \rangle = \langle \kappa_f \mid |C^{(1)} \rangle \langle \kappa_i \rangle \int_0^\infty \left[ (\mathcal{P}_f P_i + Q_f Q_i) - \frac{\omega r \pi e^2}{3a} \left( \frac{\kappa_f - \kappa_i}{2} (\mathcal{P}_f Q_i + Q_f P_i) + (\mathcal{P}_f Q_i - Q_f P_i) \right) \right] r dr ,
\]

(2.8)

\[
\langle \kappa_f \mid |\kappa_i \rangle \langle \kappa_i \rangle \int_0^\infty \left[ (\mathcal{P}_f P_i + Q_f Q_i) - \frac{\omega r \pi e^2}{3a} \left( \frac{\kappa_f - \kappa_i}{3} (\mathcal{P}_f Q_i + Q_f P_i) + (\mathcal{P}_f Q_i - Q_f P_i) \right) \right] r^2 dr ,
\]

(2.9)

and for the M1 multipole it yields

\[
\langle \kappa_f \mid |\kappa_i \rangle \langle \kappa_i \rangle \int_0^\infty \langle \kappa_f + \kappa_i \rangle \frac{\omega r \pi e^2}{a} (\mathcal{P}_f Q_i + Q_f P_i) dr ,
\]

(2.10)

where \( \kappa \)'s are the relativistic angular momentum quantum numbers, \( P \) and \( Q \) represent the radial parts of large and small components of single particle Dirac orbitals, respectively, \( \omega = \epsilon_f - \epsilon_i \) for the orbital energies \( \epsilon \)'s, \( a \) is the fine structure constant and the reduced Racah coefficients are given by

\[
\langle \kappa_f \mid |C^{(k)} \rangle \langle \kappa_i \rangle = (-1)^{j_f + 1/2} \sqrt{(2j_f + 1)(2j_i + 1)} \left( \begin{array}{ccc} j_f & k & j_i \\ 1/2 & 0 & -1/2 \end{array} \right) \pi (l_{\epsilon_f}, k, l_{\epsilon_i}) ,
\]

(2.11)
with
\[
\pi(l, m, l') = \begin{cases} 
1 & \text{for } l + m + l' = \text{even} \\
0 & \text{otherwise}.
\end{cases} 
\]  
(2.12)

The lifetime of a given state is estimated by taking the reciprocal of the total transition rates due to all possible channels \(O\), i.e. the lifetime of a state \(k\) is given by
\[
\tau_k = \frac{1}{\sum_{O,j} A_{kj}^O}. 
\]  
(2.13)

Similarly, the branching ratio of a given transition in the channel \(O\) from a state \(k\) to a lower state \(i\) is given by
\[
\Gamma_{ki}^O = \frac{\tau_i A_{ki}^O}{\sum_{O,j} A_{kj}^O} = \tau_i A_{ki}^O. 
\]  
(2.14)

The considered ion Sc III has the ground state configuration as \([3p^6]\) 3d\(_{3/2}\) which can be separated into a closed core \([3p^6]\) with the valence electron 3d\(_{3/2}\). By replacing the 3d\(_{3/2}\) valence orbital with any other excited orbital in the above configuration, the corresponding singly excited states of this ion can be obtained. In the Fock space representation, we assume a Fermi vacuum as \(|\Phi_0\rangle = [3p^6]\) and the reference state for a valence orbital \(v\) with the closed core as \(|\Phi_v\rangle = a_v^\dagger |\Phi_0\rangle\) to employ the many-body method. With these tools, the atomic state function (ASF) with a closed core and a valence orbital \(v\) in the (R)CC framework is expressed as (e.g. see [21, 28])
\[
|\Psi_v\rangle = e^T [1 + S_v]|\Phi_v\rangle, 
\]  
(2.15)

where \(T\) and \(S_v\) represent the excitation operators carrying the core–core and core–valence electron correlation effects, respectively. We consider only all possible single and double excitations (known as the CCSD method) by defining these operators in the second quantization notation as
\[
T = T_1 + T_2 = \sum_{a,\rho} a_a^\dagger a_{\rho} a_{\rho} t_{ab} + \frac{1}{4} \sum_{a, b, p, q} a_a^\dagger a_b^\dagger a_{\rho} a_{\rho} t_{ab} t_{pq}. 
\]  
(2.16)

\[ S_v = S_{1v} + S_{2v} = \sum_{\rho, \nu} a_{\rho}^\dagger a_{\nu} s_{\rho\nu}^v + \frac{1}{2} \sum_{b, p, q} a_b^\dagger a_{\rho} a_{\rho} a_{\rho} s_{\rho\rho\rho}^v. 
\]  
(2.17)

with \((a, b, c,\ldots), (p, q,\ldots)\) and \((v)\) subscripts for the second quantized operators representing core, particle (virtual) and valence orbitals, respectively. The subscripts 1 and 2 with the RCC operators correspond to the singly and doubly excited states, respectively. The \(t\) and \(s_o\) coefficients are the corresponding excitation amplitudes which are determined using the following equations:
\[
\langle \Phi_0^K | [\hat{H} e^T] | \Phi_0 \rangle = 0 
\]  
(2.18)

\[
\langle \Phi_v^K | [\hat{H} e^T] S_v | \Phi_v \rangle = -\langle \Phi_v^K | [\hat{H} e^T] | \Phi_v \rangle + \langle \Phi_v^K | S_v | \Phi_v \rangle \Delta E_v, 
\]  
(2.19)

with the superscript \(K\) representing the singly \((K = 1)\) and doubly \((K = 2)\) excited states from the corresponding reference states and the wide-hat symbol denotes the linked terms. We first obtain solutions for the amplitudes of \(T\) and use them in equation (2.19). \(\Delta E_v\) is the corresponding affinity energy of the valence electron \(v\) (also equals to negative of its ionization potential (IP)) which is evaluated simultaneously with equation (2.19) in a self-consistent approach using the following expression:
\[
\Delta E_v = \langle \Phi_v | [\hat{H} e^T] | [1 + S_v] | \Phi_v \rangle - \langle \Phi_0 | [\hat{H} e^T] | \Phi_0 \rangle. 
\]  
(2.20)

We consider the Dirac–Coulomb Hamiltonian in this calculation. Since Sc III is a medium-sized atomic system, contributions from the neglected triple and higher level excitations are expected to be small for which the considered CCSD approximation seems to be reasonable to obtain accurate results in this ion. However, we also take into account contributions from the leading order valence triple excitations by constructing operators in a perturbative approach as
\[
S_{3v} = \frac{1}{4} \sum_{b, c, p, q, r} \left( \langle O_{T2}^b c p q r | \hat{H} S_{2v}^b c p q r \rangle \langle O_{T2}^b c p q r | \hat{H} S_{2v}^b c p q r \rangle \right) \epsilon_{b, c, p, q, r}, 
\]  
(2.21)

with \(\epsilon_i\) being the DF energy of the electron in the \(i\)th orbital. It is considered as a part of the \(S_v\) operator in equation (2.20); we referred this procedure as the CCSDpT method.

The transition matrix element for a given channel \(O\) from state \(k\) to state \(i\) is evaluated by calculating the expression
\[
\frac{\langle \Psi_k | O | \Psi_i \rangle}{\sqrt{\langle \Psi_k | O | \Psi_k \rangle}} = \frac{\langle \Phi_k | [1 + S_v^k] | O | [1 + S_v^k] | \Phi_i \rangle}{\sqrt{N_i N_k}}, 
\]  
(2.22)

where \(O = e^T O e^T\) and \(N_i = \langle \Phi_i | [1 + S_v^i] | N_i | [1 + S_v^i] | \Phi_i \rangle\) with \(N = e^T e^T\). These terms involve a non-truncating series and their evaluation procedure is explained elsewhere, e.g. see [21, 28].

The trial DF wavefunction \(|\Phi_0\rangle\) is constructed initially using 32 Gaussian-type orbitals (GTOs) for each angular momentum symmetry before obtaining the self-consistent solutions. To obtain the RCC wavefunctions, 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 [18].

3. Results and discussions

We present first the IP results of various states using the DF and CCSDpT methods and compare them in table 1 with the corresponding values given in the NIST database [29]. The differences between the CCSDpT results and the NIST data are given as \(\Delta\) 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. The amount of the correlation effects in these results which are annexed through the CCSDpT method can be ascertained from the differences between the DF and CCSDpT results. An agreement between the experimental results quoted in the NIST database and CCSDpT results signifies capability of the method for obtaining the correct results in the considered system.
Table 1. IPs of different states. Differences between the CCSDpT and NIST results are given as \( \Delta \).

| State | DF (cm\(^{-1}\)) | CCSDpT (cm\(^{-1}\)) | NIST [29] (cm\(^{-1}\)) | \( \Delta \) (\%) |
|-------|----------------|----------------------|--------------------------|----------------|
| 3d \(^2\)D\(_{3/2}\) | 186 268 97 | 199 168 89 | 199 677 64 | 0.25 |
| 3d \(^2\)D\(_{5/2}\) | 186 104 28 | 198 916 43 | 199 479 73 | 0.28 |
| 4s \(^2\)P\(_{1/2}\) | 168 567 35 | 174 283 19 | 174 138 05 | 0.08 |
| 4p \(^2\)P\(_{1/2}\) | 133 649 63 | 137 631 36 | 137 573 07 | 0.04 |
| 4p \(^2\)P\(_{3/2}\) | 133 205 60 | 136 139 57 | 137 099 19 | 0.70 |
| 4d \(^2\)D\(_{3/2}\) | 50 110 93 | 87 392 72 | 87 419 75 | 0.03 |
| 4d \(^2\)D\(_{5/2}\) | 50 089 33 | 87 290 26 | 87 374 42 | 0.10 |
| 5s \(^2\)S\(_{1/2}\) | 83 029 85 | 84 743 04 | 84 814 89 | 0.08 |
| 5p \(^2\)P\(_{1/2}\) | 70 102 15 | 71 481 95 | 71 570 25 | 0.12 |
| 5p \(^2\)P\(_{3/2}\) | 69 932 66 | 71 299 70 | 71 394 22 | 0.13 |
| 4f \(^2\)F\(_{5/2}\) | 61 959 64 | 62 707 34 | 62 803 50 | 0.15 |
| 4f \(^2\)F\(_{7/2}\) | 61 960 23 | 62 707 42 | 62 803 25 | 0.15 |
| 5d \(^2\)D\(_{3/2}\) | 33 000 09 | 51 366 41 | 51 547 34 | 0.35 |
| 5d \(^2\)D\(_{5/2}\) | 32 986 18 | 51 342 51 | 51 527 23 | 0.36 |
| 6s \(^2\)S\(_{1/2}\) | 49 524 46 | 50 238 20 | 50 483 34 | 0.79 |
| 6p \(^2\)P\(_{1/2}\) | 43 206 41 | 43 837 69 | 44 187 59 | 0.79 |
| 6p \(^2\)P\(_{3/2}\) | 43 126 91 | 43 752 33 | 44 102 17 | 0.79 |

Although the calculated IP results seem to be accurate enough for considering them in the \textit{ab initio} determination of the transition properties, 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 contributions from other higher relativistic corrections in the fine-structure transitions from the QED and Breit interactions which are not considered in this 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 2, 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 not accounted here. These results can also be used to estimate the polarizabilities of different states of the considered ion. As seen from table 2, 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. The role of the correlation effects to determine these properties can be realized from the differences between the DF and CCSDpT results given in the same table. Typically, the magnitudes of the amplitudes obtained using the CCSDpT method are smaller compared to 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.

Using the transition amplitudes/strengths from the CCSDpT calculations given in table 2 and experimental wavelengths estimated from the NIST energies database (given in table 1), we determine the transition rates, emission oscillator strengths and branching ratios of various transitions.

Table 2. Calculated transition amplitudes and line strengths are given in au for different channels.

| Transition | Dirac–Fock | CCSDpT | \( S_\mu \) |
|------------|------------|--------|-------------|
| \( 3d \ 2D_{3/2} \rightarrow 4p \ 2P_{3/2} \) | \( M1 \) | 1.549 | 1.541 | 2.37 |
| | \( E2 \) | 1.934 | 1.649 | 2.72 |
| \( 4s \ 2S_{1/2} \rightarrow 3d \ 2D_{3/2} \) | \( M1 \) | 0.001 | 0.001 | 0.00 |
| | \( E2 \) | 4.051 | 3.589 | 12.88 |
| | \( E3 \) | 4.975 | 4.414 | 19.48 |
| \( 4p \ 2P_{3/2} \rightarrow 3d \ 2D_{3/2} \) | \( E1 \) | 1.535 | 1.325 | 1.76 |
| | \( E3 \) | 2.584 | 2.345 | 5.50 |
| \( 4p \ 2P_{3/2} \rightarrow 4s \ 2S_{1/2} \) | \( E1 \) | 0.683 | 0.589 | 0.35 |
| | \( E2 \) | 3.720 | 3.318 | 11.01 |
| | \( E3 \) | 1.527 | 1.514 | 1.33 |
| \( 4d \ 2D_{3/2} \rightarrow 5s \ 2S_{1/2} \) | \( M1 \) | 0.0002 | 0.0003 | 0.00 |
| | \( E1 \) | 2.811 | 2.544 | 6.47 |
| | \( E2 \) | 0.002 | 0.006 | 0.00 |
| | \( E3 \) | 1.848 | 1.678 | 2.82 |
| \( 4s \ 2S_{1/2} \rightarrow 3d \ 2D_{3/2} \) | \( M1 \) | 10.102 | 9.704 | 94.22 |
| | \( E1 \) | 3.907 | 3.719 | 13.83 |
| | \( E2 \) | 1.758 | 1.673 | 2.80 |
| \( 4d \ 2D_{3/2} \rightarrow 5p \ 2P_{3/2} \) | \( M1 \) | 0.014 | 0.015 | 0.00 |
| | \( E1 \) | 16.140 | 14.972 | 224.16 |
| \( 5s \ 2S_{1/2} \rightarrow 3d \ 2D_{3/2} \) | \( M1 \) | 0.000 | 0.000 | 0.00 |
| | \( E1 \) | 0.683 | 0.514 | 0.26 |
| | \( E2 \) | 0.844 | 0.643 | 0.41 |
| | \( E3 \) | 0.002 | 0.002 | 0.00 |
| \( 5p \ 2P_{3/2} \rightarrow 4s \ 2S_{1/2} \) | \( M1 \) | 1.453 | 1.442 | 2.08 |
| | \( E2 \) | 2.083 | 2.068 | 4.28 |
| | \( E3 \) | 0.000 | 0.000 | 0.00 |
| \( 5p \ 2P_{3/2} \rightarrow 4p \ 2P_{3/2} \) | \( M1 \) | 0.0005 | 0.0005 | 0.00 |
| | \( E2 \) | 7.734 | 7.403 | 54.80 |
| | \( E3 \) | 4.578 | 4.330 | 18.75 |
| \( 5s \ 2S_{1/2} \rightarrow 4d \ 2D_{3/2} \) | \( M1 \) | 4.949 | 4.849 | 23.51 |
Table 2. (Continued.)

| Transition | $k \rightarrow i$ | Dirac–Fock | CCSDpT | $S_{li}$ |
|------------|-------------------|-------------|---------|----------|
| 5p $^2P_{3/2}$ | $4f$ 2D$_{3/2}$ $\rightarrow$ -0.130 | -0.113 | 0.02 |
| $e_1$ | $4d$ 2D$_{3/2}$ | 0.392 | 0.340 | 0.12 |
| $e_1$ | $4s$ 2S$_{1/2}$ | -0.132 | 0.236 | 0.56 |
| $M_1$ | $4p$ 2P$_{1/2}$ | 0.005 | 0.005 | ~0 |
| $e_2$ | $4p$ 2P$_{3/2}$ | -7.540 | -7.209 | 51.97 |
| $M_1$ | $4p$ 2P$_{1/2}$ | ~0 | ~0 | ~0 |
| $e_2$ | $4p$ 2P$_{3/2}$ | -7.660 | -7.332 | 53.76 |
| $e_1$ | $4d$ 2D$_{3/2}$ | -6.124 | -5.793 | 33.56 |
| $e_1$ | $4d$ 2D$_{5/2}$ | 2.037 | 1.936 | 3.75 |
| $e_1$ | $5s$ 2S$_{1/2}$ | 7.063 | 6.851 | 46.94 |
| $M_1$ | $5p$ 2P$_{1/2}$ | 1.154 | 1.154 | 1.33 |
| $e_2$ | $5p$ 2P$_{1/2}$ | 47.408 | 45.585 | 2077.99 |
| 4f $^2P_{3/2}$ | $3d$ 2D$_{3/2}$ $\rightarrow$ -1.402 | -1.173 | 1.38 |
| $e_1$ | $3d$ 2D$_{5/2}$ | -0.376 | -0.315 | 0.011 |
| $e_1$ | $4p$ 2P$_{1/2}$ | 17.580 | 16.611 | 275.92 |
| $M_1$ | $4p$ 2P$_{1/2}$ | ~0 | ~0 | ~0 |
| $e_1$ | $4p$ 2P$_{3/2}$ | -9.471 | -8.953 | 80.16 |
| $e_1$ | $4d$ 2D$_{3/2}$ | -7.965 | -7.570 | 57.30 |
| $e_1$ | $4d$ 2D$_{5/2}$ | -2.130 | -2.025 | 4.10 |
| $e_1$ | $5p$ 2P$_{1/2}$ | -45.466 | -43.894 | 1926.68 |
| $M_1$ | $5p$ 2P$_{1/2}$ | ~0 | ~0 | ~0 |
| $e_2$ | $5p$ 2P$_{1/2}$ | -24.318 | -23.480 | 551.31 |
| 4f $^2F_{7/2}$ | $3d$ 2D$_{3/2}$ $\rightarrow$ -1.682 | -1.411 | 1.99 |
| $e_1$ | $3d$ 2D$_{5/2}$ | 23.12 | 23.20 | 538.24 |
| $e_1$ | $4p$ 2P$_{1/2}$ | -9.526 | -9.055 | 81.99 |
| $e_1$ | $4d$ 2D$_{5/2}$ | 59.16 | 59.56 | 3547.40 |
| $e_1$ | $5p$ 2P$_{1/2}$ | 1.852 | 1.852 | 3.43 |
| $M_1$ | $4f$ 2P$_{1/2}$ | 18.25 | 18.25 | 333.06 |
| 5d $^2D_{3/2}$ | $3d$ 2D$_{3/2}$ | 0.0001 | 0.000 | 0.0 |
| $e_1$ | $3d$ 2D$_{5/2}$ | -0.976 | -0.917 | 0.84 |
| $e_1$ | $3d$ 2D$_{5/2}$ | 0.0008 | 0.003 | ~0 |
| $e_1$ | $4s$ 2S$_{1/2}$ | -0.640 | -0.602 | 0.36 |
| $M_1$ | $4s$ 2S$_{1/2}$ | ~0 | ~0 | ~0 |
| $e_1$ | $4s$ 2S$_{1/2}$ | -1.856 | -1.642 | 2.70 |
| $e_1$ | $4p$ 2P$_{1/2}$ | -0.756 | -0.613 | 0.38 |
| $e_1$ | $4p$ 2P$_{1/2}$ | 0.334 | 0.270 | 0.08 |
| $M_1$ | $4d$ 2D$_{3/2}$ | ~0 | ~0 | ~0 |
| $e_1$ | $4d$ 2D$_{5/2}$ | 15.562 | 14.746 | 217.44 |
| $M_1$ | $4d$ 2D$_{5/2}$ | 0.001 | 0.003 | ~0 |
| $e_1$ | $4d$ 2D$_{5/2}$ | -0.015 | -0.015 | ~0 |
| $M_1$ | $5s$ 2S$_{1/2}$ | ~0 | ~0 | ~0 |
| $e_1$ | $5s$ 2S$_{1/2}$ | -31.762 | -31.420 | 987.22 |
| $e_1$ | $5p$ 2P$_{1/2}$ | -6.773 | -6.731 | 45.31 |
| $e_1$ | $5p$ 2P$_{1/2}$ | -3.048 | -3.030 | 9.19 |
| $e_1$ | $4f$ 2F$_{3/2}$ | -5.348 | -5.500 | 30.25 |
and present them in table 3. There are few calculations available on the transition probabilities and oscillator strengths earlier. Transition probabilities reported by us in our earlier work [18] were obtained using a lesser size configuration interaction space than the present calculation depending on the availability of the computational facility. We find consistent results from both calculations. Ali and Kim have also calculated these forbidden transition rates [16] using the multi-configuration Dirac–Fock (MCDF) method; their results are also in agreement with us except for the M1 amplitude of the 4s 2S1/2 \rightarrow 3d 2D3/2 transition. It is known that the MCDF method is not as effective as the RCC method to incorporate the core-polarization correlations comprehensively. We observe that the above M1 amplitude is about 5.12 \times 10^{-6} at the DF level and the core-polarization effects through the core correlations aggrandize it to \sim 0.001 (au) in the CCSDpT 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 wavefunctions 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 [24]. 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 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 in the determination of the lifetimes of the considered excited states 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 of the 6s and 6p states were not known earlier. In addition, we 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 for us to estimate these results due to the fact that we have calculated all possible important transition rates in this work.

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 [14] have measured lifetimes of the 4p states. Buchta et al have carried out an investigation of the lifetimes of a number of states in the considered ion using a beam-foil technique measurement with reasonable accuracies [13]. Some of the data reported by Wiese and Fuhr [24], as was mentioned in the previous paragraph, were 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 discussed above. The results are given in table 4 alongside 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 completely disaccord with the results reported in [13]. 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 of the experimental setup. We have also referred to a 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 [13]. However, this agreement may be accidental, because as is stated in the earlier paragraph, the transition amplitudes from the DF method (mean-field theory calculation) are usually larger in magnitudes compared to the results (using the length gauge expressions) obtained after inclusion of the correlation effects in the RCC method. Therefore, the mean-field results are expected to give smaller lifetime values and this is what

| Transition | Dirac–Fock | CCSDpT | S_{li} |
|------------|------------|--------|--------|
| 6p 7P3/2→ 3d 2D3/2 | E_1 | 3d 2D3/2 | \sim 0.068 | \sim 0.057 | 0.003 |
| 6p 7P3/2→ 3d 2D3/2 | E_2 | 3d 2D3/2 | 0.205 | 0.174 | 0.03 |
| 6p 7P3/2→ 4s 2S1/2 | M_1 | 4p 2P_1 | 0.002 | 0.002 | \sim 0 |
| 6p 7P3/2→ 4p 2P_1 | E_4 | 4p 2P_1 | \sim 2.092 | \sim 2.048 | 4.19 |
| 6p 7P3/2→ 4p 2P_1 | M_1 | 4p 2P_1 | \sim 0 | \sim 0 | \sim 0 |
| 6p 7P3/2→ 2.110 | E_5 | 4d 2D3/2 | 0.226 | 0.232 | 0.05 |
| 6p 7P3/2→ 4d 2D3/2 | E_6 | 4d 2D3/2 | \sim 0.678 | \sim 0.696 | 0.48 |
| 6p 7P3/2→ 5s 2S1/2 | M_1 | 5p 2P_1 | 0.005 | 0.005 | \sim 0 |
| 6p 7P3/2→ 5p 2P_1 | E_8 | 5p 2P_1 | \sim 23.928 | \sim 22.998 | 528.90 |
| 6p 7P3/2→ 5p 2P_1 | M_1 | 5p 2P_1 | \sim 0 | 0.003 | \sim 0 |
| 6p 7P3/2→ 24.295 | E_9 | 5p 2P_1 | 23.368 | 546.06 |
| 6p 7P3/2→ 4f 2F7 | M_1 | 4f 2F7 | \sim 0 | \sim 0 | \sim 0 |
| 6p 7P3/2→ 9.998 | E_10 | 4f 2F7 | \sim 9.852 | 97.06 |
| 6p 7P3/2→ 4f 2F7 | E_11 | 4f 2F7 | 24.489 | 24.131 | 582.26 |
| 6p 7P3/2→ 3d 2D3/2 | E_12 | 5d 2D3/2 | 3.830 | 3.636 | 13.22 |
| 6p 7P3/2→ 5d 2D3/2 | E_13 | 5d 2D3/2 | \sim 11.506 | \sim 10.928 | 119.42 |
| 6p 7P3/2→ 6s 2S1/2 | M_1 | 6p 2P_1 | \sim 11.676 | \sim 11.522 | 132.76 |
| 6p 7P3/2→ 6p 2P_1 | E_14 | 6p 2P_1 | \sim 1.154 | \sim 1.154 | 1.33 |
| 6p 7P3/2→ 133.050 | E_15 | 6p 2P_1 | \sim 129.491 | 16.641.00 |
Table 3. Wavelengths (λ in Å), transition rates (A in s⁻¹), oscillator strengths (f) and branching ratios (Γ) from different works. Numbers given as [l] implies $10^l$.

| Upper state (k) | Lower state (l) | $\lambda_{kl}$ | $A_{kl}^{O}$ Others | $f_{kl}^{O}$ Others | $\Gamma_{kl}^{O}$ Present |
|-----------------|-----------------|----------------|---------------------|---------------------|--------------------------|
| 3d$\frac{5}{2}$ $\rightarrow$ 3d$\frac{1}{2}$ | 505 970.4 | 8.32[−5]$^b$ 8.32[−5]$^b$ 8.24[−5]$^b$ | 8.33[−5] | ~0 | ~1.0 |
| 3d$\frac{5}{2}$ $\rightarrow$ 3d$\frac{1}{2}$ | 3915.53 | 1.75[−1]$^b$ 1.53[−1]$^b$ | 1.53[−1] | ~0 | ~0.0 |
| 4s$\frac{1}{2}$ $\rightarrow$ 3d$\frac{3}{2}$ | 3946.07 | 1.15$^c$ 11.9$^b$ 11.41$^c$ | 7.83 | ~0 | 0.407 |
| 4p$\frac{1}{2}$ $\rightarrow$ 3d$\frac{3}{2}$ | 1610.194 | 4.4[8]$^d$ 4.26[8] | 0.085$^d$ 0.083 0.389 |
| 4p$\frac{3}{2}$ $\rightarrow$ 3d$\frac{3}{2}$ | 1598.00 | 4.6[7]$^d$ 4.31[7] | 0.018$^d$ 0.017 0.060 |
| 4d$\frac{3}{2}$ $\rightarrow$ 3d$\frac{3}{2}$ | 890.81 | 7.95$^c$ 8.21$^b$ 7.86 | 7.83 | ~0 | 0.407 |
| 5s$\frac{1}{2}$ $\rightarrow$ 3d$\frac{3}{2}$ | 2012.91 | 9.18$^d$ | ~0 | ~0.0 |
| 4d$\frac{5}{2}$ $\rightarrow$ 3d$\frac{3}{2}$ | 890.45 | 0.003 | ~0 | ~0.0 |
| 5s$\frac{1}{2}$ $\rightarrow$ 3d$\frac{3}{2}$ | 870.61 | 2.87$^d$ | ~0 | ~0.0 |
| 4d$\frac{1}{2}$ $\rightarrow$ 3d$\frac{3}{2}$ | 872.11 | 2.87[−3] | ~0 | ~0.0 |
| 5s$\frac{1}{2}$ $\rightarrow$ 3d$\frac{3}{2}$ | 38 389.78 | 3.43[−9] | ~0 | ~0.0 |
| 5s$\frac{1}{2}$ $\rightarrow$ 3d$\frac{3}{2}$ | 39 069.67 | 5.86$^d$ | ~0 | ~0.0 |
Table 3. (Continued.)

| Upper state (k) | Lower state (i) | $\lambda_{ki}$ | $A_{ki}^O$ | $f_{ki}^O$ | $\Gamma_{ki}^O$ |
|-----------------|-----------------|---------------|------------|-----------|--------------|
|                 |                 |               | Others     | Present   | Others       | Present       | Present       |
| $5p_{1/2}$      | $E_1$           | 780.60        | 1.5[8]$^d$ | 1.35[8]   | 0.0066$^d$  | 0.006         | 0.448         |
|                 | $E_1$           | 974.97        | 3.51[7]    |            | 0.005       | 0.116         |
|                 | $M_1$           | 1515.09       | $^\sim$0   | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $M_1$           | 1526.04       | 0.113      | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_2$           | 3.71[3]       |            | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_1$           | 4d$_{3/2}$    | 6309.35    | 7.0[7]$^d$ | 7.56[7]    | 0.21$^d$      | 0.226         | 0.251         |
|                 | $E_2$           | 5s$_{1/2}$    | 7550.22    | 5.4[7]$^d$ | 5.53[7]    | 0.47$^d$      | 0.473         | 0.184         |
| $5p_{3/2}$      | $E_1$           | 779.53        | 1.5[7]$^d$ | 1.38[7]    | 0.0014$^d$  | 0.001         | 0.046         |
|                 | $E_1$           | 780.73        | 1.3[8]$^d$ | 1.23[8]    | 0.0079$^d$  | 0.007         | 0.407         |
|                 | $E_1$           | 973.29        | 3.07[7]    |            | 0.009       | 0.101         |
|                 | $M_1$           | 1511.06       | 0.005      | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_2$           | 1.85[3]       |            | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $M_1$           | 1521.95       | 5.92[−5]   | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_2$           | 1.84[3]       |            | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_1$           | 4d$_{3/2}$    | 6240.04    | 7.72[6]$^d$| 7.74[6]    | 0.042$^d$     | 0.045         | 0.026         |
|                 | $E_1$           | 6257.74       | 6.5[7]$^d$ | 6.94[7]    | 0.25$^d$    | 0.272         | 0.229         |
|                 | $M_1$           | 7451.19       | 5.7[7]$^d$ | 5.75[7]    | 0.94$^d$    | 0.957         | 0.190         |
|                 | $E_1$           | 5p$_{1/2}$    | 568.085.0  | 4.90[−5]   | $^\sim$0   | $^\sim$0      |
|                 | $E_1$           | 983[−9]       |            | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $M_1$           | 1521.96       | 5.92[−5]   | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_2$           | 1.84[3]       |            | $^\sim$0   | $^\sim$0   | $^\sim$0      |
| $4f_{3/2}$      | $E_1$           | 730.60        | 1.1[9]$^d$ | 1.19[9]    | 0.13$^d$    | 0.143         | 0.751         |
|                 | $E_1$           | 731.66        | 7.8[7]$^d$ | 8.59[7]    | 0.0062$^d$  | 0.007         | 0.051         |
|                 | $E_2$           | 337.443       | 1.20[4]    |            | $^\sim$0   | $^\sim$0      |
|                 | $M_1$           | 1345.97       | 2.56[−6]   | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_2$           | 3.39[3]       |            | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_1$           | 4d$_{3/2}$    | 4062.36    | 2.9[8]$^d$ | 2.89[8]    | 1.1$^d$       | 1.072         | 0.182         |
|                 | $E_1$           | 4069.85       | 2.1[7]$^d$ | 2.05[7]    | 0.052$^d$   | 0.051         | 0.013         |
|                 | $E_2$           | 5p$_{1/2}$    | 11 406.74  | 1.862      | $^\sim$0   | $^\sim$0      |
|                 | $E_2$           | 11 640.47     | 1.35[−11]  | $^\sim$0   | $^\sim$0   | $^\sim$0      |
| $4f_{1/2}$      | $E_1$           | 731.65        | 1.1[9]$^d$ | 1.29[9]    | 0.12$^d$    | 0.138         | 0.807         |
|                 | $E_2$           | 1345.97       | 1.71[4]    |            | $^\sim$0   | $^\sim$0      |
|                 | $E_1$           | 4d$_{3/2}$    | 4069.81    | 3.1[8]$^d$ | 3.08[8]    | 1.0$^d$       | 1.021         | 0.192         |
|                 | $E_2$           | 11 640.13     | 2.323      | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $M_1$           | 4f$_{3/2}$    | 4.00[8]    | 1.81[−13]  | $^\sim$0   | $^\sim$0      |
|                 | $E_2$           | 4.55[−24]     |            | $^\sim$0   | $^\sim$0   | $^\sim$0      |
| $5d_{3/2}$      | $M_1$           | 676.58        | 3.46[−3]   | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_2$           | 1954.32       | 1.66[3]    |            | $^\sim$0   | $^\sim$0      |
|                 | $M_1$           | 677.74        | 710.019    | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_2$           | 827.02        | 2.93[−4]   | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_2$           | 1.95[3]       |            | $^\sim$0   | $^\sim$0   | $^\sim$0      |
|                 | $E_1$           | 4p$_{3/2}$    | 1159.22    | 1.6[8]$^d$ | 1.22[8]    | 0.067$^d$     | 0.050         | 0.312         |
|                 | $E_1$           | 1179.62       | 3.2[7]$^d$ | 2.25[7]    | 0.0066$^d$  | 0.005         | 0.057         |
Table 3. (Continued.)

| Upper state (k) | Lower state (l) | $\lambda_{kl}$ | $\alpha_{kl}^O$ Others | Present | $\beta_{kl}^O$ Others | Present | $\Gamma_{kl}^O$ Others | Present |
|-----------------|-----------------|-----------------|------------------------|---------|------------------------|---------|------------------------|---------|
| $M^1_1$ 4d$_{3/2}$ | 2775.75 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^2_2$ 4d$_{3/2}$ | 369.313 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $M^3_1$ 4d$_{5/2}$ | 2783.66 | 2.09 [−4] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^3_2$ 4d$_{5/2}$ | 2783.67 | 157.227 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $M^5_1$ 5s$_{1/2}$ | 2996.10 | 9.03 [−7] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^5_2$ 5s$_{1/2}$ | 1.14 [3] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^1_1$ 5p$_{1/2}$ | 4971.28 | 1.8 [8]$^d$ | 1.8 [8] | 1.4$^d$ | 1.386 | 0.479 | 0.479 | 0.479 |
| $E^1_1$ 5p$_{3/2}$ | 5016.73 | 3.6 [7]$^d$ | 3.6 [7] | 0.14$^d$ | 0.139 | 0.094 | 0.094 | 0.094 |
| $E^1_1$ 4f$_{5/2}$ | 8817.62 | 2.1 [7]$^d$ | 2.23 [7] | 0.16$^d$ | 0.173 | 0.057 | 0.057 | 0.057 |
| 5d$_{5/2}$ | $M^1_1$ 3d$_{3/2}$ | 674.99 | 0.004 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^2_2$ 3d$_{3/2}$ | 479.243 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $M^3_1$ 3d$_{5/2}$ | 675.89 | 0.494 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^3_2$ 3d$_{5/2}$ | 2.2 [3] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^1_1$ 4s$_{1/2}$ | 815.59 | 2.11 [3] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^1_1$ 4p$_{1/2}$ | 1168.61 | 1.9 [8]$^d$ | 1.40 [8] | 0.060$^d$ | 0.043 | 0.368 | 0.368 | 0.368 |
| $M^1_1$ 4d$_{3/2}$ | 2786.09 | 1.50 [−5] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^2_2$ 4d$_{3/2}$ | 103.18 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $M^5_1$ 4d$_{5/2}$ | 2789.62 | 6.55 [−3] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^5_2$ 4d$_{5/2}$ | 413.268 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| 6s$_{1/2}$ | $E^1_1$ 5s$_{1/2}$ | 3004.12 | 1.13 [3] | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^1_1$ 5p$_{1/2}$ | 5033.47 | 2.2 [8]$^d$ | 2.18 [8] | 1.2$^d$ | 1.242 | 0.573 | 0.573 | 0.573 |
| $E^1_1$ 4f$_{3/2}$ | 8868.18 | 0.996 [6]$^d$ | 1.04 [6] | 0.01$^d$ | 0.012 | 0.023 | 0.023 | 0.023 |
| $E^1_1$ 4f$_{5/2}$ | 8868.38 | 2.0 [7]$^d$ | 2.09 [7] | 0.18$^d$ | 0.185 | 0.055 | 0.055 | 0.055 |
| $M^1_1$ 5d$_{3/2}$ | 4972.650 | 8.78 [−8] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^2_2$ 5d$_{3/2}$ | 1.57 [−13] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $M^1_1$ 3d$_{3/2}$ | 670.27 | 2.07 [−3] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^2_2$ 3d$_{3/2}$ | 1.54 [2] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^2_2$ 4s$_{3/2}$ | 671.16 | 237.108 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $M^1_1$ 4s$_{1/2}$ | 808.70 | 6.53 [−2] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^1_1$ 4p$_{1/2}$ | 1148.24 | 1.23 [8] | 0.024 | 0.201 | 0.201 | 0.201 | 0.201 | 0.201 |
| $E^1_1$ 4p$_{3/2}$ | 1154.52 | 2.48 [8] | 0.025 | 0.406 | 0.406 | 0.406 | 0.406 | 0.406 |
| $M^1_1$ 4d$_{5/2}$ | 2707.36 | 6.8 [−6] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^2_2$ 4d$_{5/2}$ | 156.908 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| 6p$_{1/2}$ | $E^1_1$ 3d$_{3/2}$ | 2710.68 | 236.973 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^2_2$ 3d$_{3/2}$ | 2912.77 | 5.46 [−4] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^1_1$ 5s$_{1/2}$ | 4742.28 | 7.78 [7] | 0.262 | 0.127 | 0.127 | 0.127 | 0.127 | 0.127 |
| $E^1_1$ 5p$_{1/2}$ | 4782.20 | 1.62 [8] | 0.278 | 0.265 | 0.265 | 0.265 | 0.265 | 0.265 |
| $M^1_1$ 5d$_{3/2}$ | 93.984 | 3.09 [−11] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^2_2$ 5d$_{3/2}$ | 51.11 [−4] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^1_1$ 5d$_{5/2}$ | 95.795 | 6.98 [−4] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^1_1$ 3d$_{5/2}$ | 643.13 | 6.27 [7] | 0.002 | 0.397 | 0.397 | 0.397 | 0.397 | 0.397 |
| $E^2_2$ 4s$_{3/2}$ | 769.52 | 2.96 [7] | 0.003 | 0.187 | 0.187 | 0.187 | 0.187 | 0.187 |
| $M^1_1$ 4p$_{1/2}$ | 1070.83 | 4.40 [−4] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^1_1$ 4p$_{3/2}$ | 1076.29 | 0.009 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^2_2$ 4p$_{3/2}$ | 1.67 [3] | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 | ~0 |
| $E^1_1$ 4d$_{3/2}$ | 2313.09 | 2.15 [7] | 0.009 | 0.136 | 0.136 | 0.136 | 0.136 | 0.136 |
by Buchta for Sc III in this work are more precise than the measurements therefore, appears that the estimated lifetimes of the 4p states results agreeing with their corresponding measured values. It, shown the importance of the correlation effects to obtain these further measurements of the lifetimes of different states in et al have brought up another example of how the measured approximated many-body theory. Furthermore, Buchta converged amplitudes than the velocity gauge expressions in this ion using the modern advanced experimental techniques to probe their accuracies and test the potential of different many-body methods to reproduce them.

The lifetime of the 5s state and the oscillator strength of the 4p–5s transition in Sc III were reported as 1.4(2) ns and 0.13(2) in [13], which we obtain as 1.08(2) ns and 0.168, respectively. Our oscillator strength for the above transition also matches reasonably with the tabulated result as 0.15 in [13]. The measured oscillator strength for the 3d → 4f transition is reported to be 0.03 [13] which differs substantially from our result 0.14; but our result agrees with the results reported in [24]. With all the analysis, it seems that the reported results in this work are more accurate and can be used reliably in any other applications.

is obtained in the mean-field theory calculation. It should also be noted that the length gauge expressions give faster converged amplitudes than the velocity gauge expressions in an approximated many-body theory. Furthermore, Buchta et al have brought up another example of how the measured lifetimes of the 4p states in the calcium ion (Ca II) are also closer to the calculations using the velocity gauge expressions than the length gauge expressions. In fact, we have also studied the lifetimes of various states using the length gauge expressions in Ca II using our CCSDpT method [22, 31] and shown the importance of the correlation effects to obtain these results agreeing with their corresponding measured values. It, therefore, appears that the estimated lifetimes of the 4p states for Sc III in this work are more precise than the measurements by Buchta et al [13]. It would be appropriate to carry out further measurements of the lifetimes of different states in this ion using the modern advanced experimental techniques to probe their accuracies and test the potential of different many-body methods to reproduce them.

### Table 3. (Continued.)

| Upper state (k) | Lower state (i) | \( \lambda_{ki} \) | \( A_{ki}^\text{O} \) | \( f_{ki}^\text{O} \) | \( \Gamma_{ki}^\text{O} \) |
|-----------------|----------------|-----------------|-----------------|-----------------|-----------------|
|                 |                | Others Present  | Others Present  | Others Present  | Others Present  |
| 6p3/2           | 5s3/2          | 2461.40         | 5.99[5]         | 0.0005          | 0.004           |
|                 | 5p3/2          | 3651.94         | 4.43[-5]        | ~0              | ~0              |
|                 | 5p3/2          | 3675.58         | 6.04[-3]        | ~0              | ~0              |
|                 | 5p3/2          | 3675.58         | 465.653         | ~0              | ~0              |
|                 | 4f5/2          | 5371.75         | 43.43           | ~0              | ~0              |
|                 | 5d5/2          | 13 587.42       | 2.69[7]         | 0.372           | 0.170           |
|                 | 6s5/2          | 15 883.73       | 1.68[7]         | 0.635           | 0.106           |
|                 | 3d3/2          | 642.78          | 6.41[6]         | 0.0004          | 0.040           |
|                 | 3d3/2          | 643.59          | 5.75[7]         | 0.002           | 0.363           |
|                 | 4s3/2          | 769.02          | 2.68[7]         | 0.005           | 0.169           |
|                 | 4p1/2          | 1069.85         | 0.003           | ~0              | ~0              |
|                 | 4p1/2          | 837.868         | ~0              | ~0              |
|                 | 4p1/2          | 1075.3          | 0.010           | ~0              | ~0              |
|                 | 4p1/2          | 1.32[3]         | ~0              | ~0              |
|                 | 4d3/2          | 2308.53         | 2.22[6]         | 0.002           | 0.014           |
|                 | 4d3/2          | 2310.95         | 1.99[7]         | 0.011           | 0.126           |
|                 | 5s3/2          | 2456.24         | 3.55[5]         | 0.0006          | 0.002           |
|                 | 5p1/2          | 3640.59         | 4.59[-3]        | ~0              | ~0              |
|                 | 5p1/2          | 231.479         | ~0              | ~0              |
|                 | 5p1/2          | 3664.07         | 1.23[-3]        | ~0              | ~0              |
|                 | 5p1/2          | 2.31[2]         | ~0              | ~0              |
|                 | 5p3/2          | 5347.21         | 4.41[-11]       | ~0              | ~0              |
|                 | 4f5/2          | 6.21[1]         | ~0              | ~0              |
|                 | 4f7/2          | 5347.28         | 3.72[1]         | ~0              | ~0              |
|                 | 5d5/2          | 13 467.90       | 2.48[7]         | 0.451           | 0.157           |
|                 | 5d5/2          | 13 431.53       | 2.76[6]         | 0.075           | 0.017           |
|                 | 6s5/2          | 15 671.11       | 1.75[7]         | 1.289           | 0.110           |
|                 | 6p1/2          | 1170 686.0      | 5.60[-6]        | ~0              | ~0              |
|                 | 6p1/2          | 2.13[-9]        | ~0              | ~0              |

References a[15]; b[16]; c[18]; d[24].
Using the forbidden transition amplitudes, we find very large lifetimes for the $3d^2D_{3/2}$ and $4s^2S_{1/2}$ states. The lifetime of the $3d^2D_{3/2}$ state is found to be $12\,\text{135}s$ which is very large; it is due to the highly forbidden transition between the corresponding fine structure states with very small $E\text{E}$. The lifetime of the $4s^2S_{1/2}$ state is found to be $0.05s$ which is also large enough in an atomic scale so that it can be used to carry out any precision experiments with this state. These results are also in perfect agreement with our previous findings [18].

### 4. 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 16 states in this ion. We have compared our results with the previously reported ones and find a reasonable 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 the scandium element. Furthermore, these results can also be directive for the new experiments to affirm the accuracies of the reported properties.

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### Table 4. Lifetimes ($\tau$) of low-lying states in Sc III.

| State      | This work | Others          | Experiments |
|------------|-----------|-----------------|-------------|
| $3d^2D_{3/2}$ | 12 135(100) | 12 130.86$^a$ |             |
| $4s^2S_{1/2}$ | 0.05(1)   | 0.0519$^e$     |             |

Lifetimes in ns

| Transition | $\tau$ (ns) |
|------------|-------------|
| $4p^3P_{1/2}$ | 1.43(2) |
| $4p^3P_{3/2}$ | 1.04(3) |
| $4d^2D_{3/2}$ | 0.95(1) |
| $5s^2S_{1/2}$ | 1.08(2) |
| $5p^3P_{1/2}$ | 3.32(2) |
| $5p^3P_{3/2}$ | 3.31(3) |
| $4f^3P_{3/2}$ | 0.61(1) |
| $4f^3F_{5/2}$ | 0.63(2) |
| $5d^2D_{3/2}$ | 2.56(1) |
| $5p^2P_{3/2}$ | 6.32(9) |
| $6s^2S_{1/2}$ | 1.66(1) |
| $6p^2P_{1/2}$ | 3.5(8)$^a$ |
| $6p^2P_{3/2}$ | 3.5(8)$^a$ |

References: $^a$[18]; $^b$[14]; $^c$[30]; $^d$[13].