Theoretical spectroscopic studies of the atomic transitions and lifetimes of low-lying states in Ti IV

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Abstract
The astrophysically important electric quadrupole (E2) and magnetic dipole (M1) transitions for the low-lying states of triply ionized titanium (Ti IV) are calculated very accurately using a state-of-the-art all-order many-body theory called coupled cluster (CC) method in the relativistic framework. Different many-body correlations of the CC theory has been estimated by studying the core and valence electron excitations to the unoccupied states. The calculated excitation energies of different states are in excellent agreement with the measurements. Also, we compare our calculated electric dipole (E1) amplitudes of few transitions with recent many-body calculations by others. The lifetimes of the low-lying states of Ti IV have been estimated and long lifetime is found for the first excited 3d²D₅/₂ state, which suggested that Ti IV may be one of the useful candidates for many fundamental studies of physics. Most of the forbidden transition results reported here are not available in the literature, to the best of our knowledge.

1. Introduction
With the advent of improved technologies in observational astronomy, laboratory plasma and atomic research, the study of weak signals in high resolution spectrum has become frontline research. However, in many of the cases experimental measurements are difficult, especially for forbidden transitions of stripped electronic systems. Whereas these transitions are very important in various fields of science and technology and detail requirements of their accurate transition rates are discussed in the following part of this paper.

The forbidden lines provide important clues in areas of astrophysics, because of the long lifetime of the upper state against radiative decay [1]. These lines are particularly sensitive to the collisional de-excitations and serve as indicators of electron density and temperature in the emission region in astrophysics [2, 3] and laboratory tokamak plasma [4]. Also they are commonly observed in the solar corona, quasars and gaseous nebulae with an intensity often comparable to accompanying allowed transition lines [5]. Many astrophysical phenomena such as coronal heating, evolution of chemical composition in stellar envelopes, determination of the chemistry in the envelope of planetary nebulae precursor are believed to be explained largely by these forbidden lines [6, 7].

Titanium (Ti) is observed in a variety of stellar objects, like in the Sun where Ti figures third place in terms of number of lines [8]. Various ionization stages of Ti are present in stellar plasma, for instance in the τ Sco spectrum [9]. Recently, the emission lines of triply ionized titanium (Ti IV) have been detected in Wolf-Rayet star [10]. Ti IV in oxidized form, used in dark and photo-induced decomposition of ozone in air, has also been studied [11].

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Accurate estimations of the forbidden transitions of this ionized system are necessary to explain and quantify the band structure of the energy level of this system doped in crystal materials. Doping of Ti IV in crystal materials is used to build optical and polymer devices [12]. The spark spectrum [13] and patronization studies [14] of Ti IV provide the excitations energies and spontaneous transition spectrum \([13]\) and patronization studies \([14]\) of Ti IV is used to build optical and polymer devices \([12]\). The crystal materials. Doping of Ti IV in crystal materials is necessary to explain and quantify the valence electrons correlation contributions obtained from the tiny effects in fundamental physics have been considered by to study sophisticated problems \([16, 17]\) of various precise perturbative in nature and its relativistic extension has been computed forbidden transitions among the low-lying states of Ti IV using Dirac–Coulomb spin orbitals. The CC theory is non-via the valence-universal wave-operator \(\Omega\) \([24, 21]\) written in the normal ordered form as

\[
\Omega = \{\exp(\mathcal{S})\},
\]  

(2.2)

where \(\mathcal{S} = \sum_{k=0}^{\infty} \sum_{l=0}^{n} S(k,l) = S^{(0,0)} + S^{(0,1)} + S^{(1,0)} + \cdots\),

(2.3)

Here \([\cdots]\) stands for the normal ordering of the creation and annihilation operators defined with respect to the Dirac–Fock (DF) wavefunction of the closed-shell system. For example, the normal ordered form of the Dirac–Coulomb Hamiltonian used here is given by

\[
\mathcal{H} = H - \langle \Phi | H | \Phi \rangle = H - E_{DF} = \sum_{ij} [\hat{a}_i^{\dagger} \hat{a}_j] \{a_i^\dagger a_j\}
\]

(2.4) where

\[
(i j || kl) = (i j) \frac{1}{r_{12}} |kl| - (i j) \frac{1}{r_{12}} |lk|.
\]

(2.5)

Here \(E_{DF}\) is the DF energy, \(f\) is the one-electron Fock operator, \(a_i^\dagger (a_i)\) is the annihilation (creation) operator (with respect to the DF state as the vacuum) for the \(i\)th electron.

At this juncture, it is convenient to single out the core-cluster amplitudes \(S^{(0,0)}\) and let us call them \(T_i\). The rest of the cluster amplitudes will henceforth be called as \(S_i\). Since \(\Omega\) corresponding to the valence orbital \(v\) is in normal order, we can rewrite equation (2.2) as

\[
\Omega = \exp(T) \{\exp(S)v\} = \Omega, \Omega_v.
\]

(2.6)

Now, if we define

\[
H_{eff} = P^{(k,l)} \Omega, P^{(k,l)},
\]

(2.7)

with the operator \(P^{(k,l)}\) being the model space projector for \(k\)-hole and \(l\)-particle, which satisfies complete model space condition. The ‘valence-universal’ wave-operator \(\Omega\) in equation (2.6) is parametrized in such a way that the states generated by its action on the reference space satisfy the Fock-space Bloch equation

\[
H \Omega P^{(k,l)} = \Omega P^{(k,l)} H_{eff} P^{(k,l)},
\]

(2.8)

To formulate the theory for direct energy differences, we premultiply equation (2.8) by \(e^{-T}\) and get

\[
\Omega (e^{S} ) P^{(k,l)} = (e^{S} ) P^{(k,l)} H_{eff} P^{(k,l)}, \quad (k, l) \neq (0, 0),
\]

(2.9)

where \(\Omega = e^{-T} H e^{T}\). Since \(\Omega\) can be parametrized using the Wick’s theorem into a connected operator \(\hat{H}\) and \(E_{ref gyr}\) (\(N\)-electron closed-shell reference or ground-state energy), we likewise define \(H_{eff}\) as

\[
H_{eff} = \hat{H}_{eff} + E_{ref gyr}.
\]

(2.10)

Substituting equation (2.10) into equation (2.9), we obtain the Fock-space Bloch equation for energy differences:

\[
\hat{H} (e^{S} ) P^{(k,l)} = (e^{S} ) P^{(k,l)} \hat{H}_{eff} P^{(k,l)}.
\]

(2.11)
Equations (2.8) and (2.11) are solved by Bloch projection method, involving the left projection of the equation with $P^{(k,t)}_{\alpha}$ and its orthogonal complement $Q^{(k,t)}_{\beta}$. To obtain the effective Hamiltonian and the cluster amplitudes, respectively.

In this work, we first solve the Fock-space CC for $k = l = 0$ to obtain the $T$ amplitudes, which construct $H_{\text{eff}}$. Equation (2.11) for $k = 0, l = 1$ is solved to determine the $S_e$ amplitudes. The Hamiltonian constructed from $H$, $T$, and $S_e$ is then diagonalized within the model space to obtain the desired eigenvalues and eigenvectors [23].

In this paper, effects of triple excitations are included in the open-shell CC amplitudes which correspond to the correlation to the valence orbitals, by an approximation that is similar in spirit to CCSD(T) [25]. The approximate valence triple excitation amplitude is given by

$$S_{v}^{pq,r} = \frac{(VS_{2}V)_{pq,r}}{e_a + e_b + e_k - e_p - e_q - e_r}. \quad (2.12)$$

where $S_{v}^{pq,r}$ are the amplitudes corresponding to the simultaneous excitation of orbitals $a, b, k$ to $p, q, r$, respectively; $VS_{2}$ and $V$ are the connected composites involving $V$ and $T$, and $V$ and $S^{(0,1)}$, respectively, where $V$ is the two electron Coulomb integral and $e’s$ are the orbital energies.

3. Computational procedure

The transition matrix element due to any operator $D$ is evaluated in the CC method by expressing it as

$$D_{fi} = \langle \Psi_f | D | \Psi_i \rangle \frac{\langle \Psi_f | (1 + \hat{S})^{1} | \Psi_i \rangle}{\sqrt{\langle \Psi_f | S | \Psi_i \rangle}}.$$ \hspace{1cm} (3.1)

Here, only consideration comes from the single power of $S^{(0,1)}$ operator with $S^{(0,1)}_1$ and $S^{(0,1)}_2$ representing single excitation operators from the valence orbital and double excitations from core-valence orbitals, respectively. Interesting correlation features of the transition operator $D$ are found in the contraction of $\mathcal{D} = e^{\dagger}De^{\dagger}$ with $S^{(0,1)}_1$ and $S^{(0,1)}_2$, which represents single excitation operators from valence orbital and double excitations from core-valence orbitals, respectively. Since the considered system is a single valence system, only one power of the $S^{(0,1)}$ operator will contribute in the CCSD(T) calculation.

For computational simplicity, we express $\mathcal{D}$ as effective terms using the generalized Wick’s theorem [20] as

$$\mathcal{D} = (e^{\dagger}De^{\dagger})_{1,1} + (e^{\dagger}De^{\dagger})_{1,2} + (e^{\dagger}De^{\dagger})_{2,2} + \ldots. \quad (3.2)$$

where we have used the abbreviations f.c., o.b. and t.b. for fully contracted, effective one-body and effective two-body terms, respectively. In this expansion of $\mathcal{D}$, the effective one-body and two-body terms are computed keeping only terms of the form

$$\mathcal{D}_{1,2} = D + T^{1}D + DT^{1}DT^{1}, \quad (3.3)$$

and

$$\mathcal{D}_{1,2} = DT_{1} + T^{1}D + DT_{2} + T^{1}DT^{1}, \quad (3.4)$$

respectively. Other effective terms correspond to higher orders in the residual Coulomb interaction and hence they are neglected in the present calculation.

The reduced matrix elements corresponding to $E1, E2$ and $M1$ transitions are given in our earlier papers [26, 27]. The emission transition probabilities $(in s^{-1})$ for the $E1, E2$ and $M1$ channels from states $f$ to $i$ are given by

$$A_{fi}^{E1} = \frac{2.0261 \times 10^{18}}{\lambda_{[f]}[j]} S^{E1} \quad (3.5)$$

$$A_{fi}^{E2} = \frac{1.1995 \times 10^{18}}{\lambda_{[j]}[j]} S^{E2} \quad (3.6)$$

$$A_{fi}^{M1} = \frac{2.6973 \times 10^{13}}{\lambda^{2}[j]} S^{M1}, \quad (3.7)$$

where $[j] = 2j + 1$ is the degeneracy of a f state, $S$ is the square of the transition matrix elements of any of the corresponding transition operator $D$ and $\lambda$ (in Å) are the corresponding transition wavelength.

4. Result and discussions

Many-body calculations started with the closed-shell coupled cluster calculations of Ti V. The reference state of this closed-shell system is obtained from the Dirac–Fock (DF) calculation using the Gaussian-type orbitals (GTO) formalism [28]. The exponent of the GTO functions are obtained from the universal even tempering condition with $\alpha = 0.00825$ and $\beta = 2.73$ for all the symmetries. The number of basis functions used in this DF calculations are 32, 30, 25, 20, 20 for $l = 0, 1, 2, 3, 4$ symmetries. Number of DF orbitals corresponding to these symmetries used in the closed-shell CC calculations are 11, 9, 8, 8 and 6. Number of active orbitals for different symmetries used in these calculations are based on the convergent criteria of core correlation energies for which it satisfies the numerical completeness.

In Table 1, we have given the excitation energies obtained using the CCSD(T) method of a few low-lying excited states considering $3d_{3/2}$ as a ground state. Kingston and Hibbert [15] have also calculated few of them by using the multiconfiguration (CIV3) method. Our calculated results are in better agreement with the experimental results (obtained from National Institute of Standard and Technology (NIST) [29]) in comparison with the CIV3 results. Except for $3d_{3/2}$ state, the average deviation with the NIST results are only 0.427%, whereas in the CIV3 method it is around 1.08%. The CC-calculated fine structure splitting (FS) of $3d$ state has far better agreement than the CIV3 calculation. Also, the excellent agreement with the experiment of the FS splittings of $F$ states indicates the accurate description of correlation in the present CC approach, especially all order considerations of core-polarization and pair-correlation effects. Though the agreement with the experiment of our FS result for $5f$ state is almost exact, but the ordering differs. The splitting energy is so
The millisecond lived excited 4s state might be plasma temperature diagnostics in stars and plasma fusion. It is worthy to do further study.

Table 1. Excitation energies (EE) in cm$^{-1}$ of different levels of Ti IV and its comparison with NIST value and CIV3 values and the fine structure splitting (FSS). Since the CIV3 results reported in the reference are in au, we have rounded them off to the integral figures in cm$^{-1}$.

| States  | NIST   | CIV3   | CC   |
|---------|--------|--------|------|
| 3d$_{3/2}$ | 382.10 | 0      | 0    |
| 3d$_{5/2}$ | 388.92 | 439    | 418.02 |
| 4s$_{1/2}$ | 127.921 | 124.750 | 128.769 |
| 4p$_{1/2}$ | 128.739 | 125.540 | 128.534 |
| 4p$_{3/2}$ | 196.804 | 196.964 | 197.050 |
| 4d$_{3/2}$ | 196.889 | 97.050 | 85.69 |
| 5s$_{1/2}$ | 212.407 | 212.823 | 231.061 |
| 5p$_{1/2}$ | 230.608 | 228.715 | 231.061 |
| 5p$_{3/2}$ | 230.924 | 228.978 | 231.444 |
| 4f$_{5/2}$ | 236.135 | 234.882 | 236.217 |
| 4f$_{7/2}$ | 236.142 | 234.882 | 236.220 |
| 5d$_{5/2}$ | 258.838 | 259.373 | 259.419 |
| 5d$_{3/2}$ | 258.877 | 259.373 | 259.419 |
| 6s$_{1/2}$ | 265.847 | 266.256 | 266.256 |
| 6p$_{1/2}$ | 274.726 | 272.720 | 275.396 |
| 6p$_{3/2}$ | 274.881 | 272.829 | 275.620 |
| 5f$_{5/2}$ | 275.847 | 276.670 | 277.647 |
| 5f$_{7/2}$ | 275.861 | 272.675 | 277.633 |
| 5g$_{7/2}$ | 278.510 | 278.530 | 278.531 |
| 5g$_{9/2}$ | 278.511 | 278.531 | 278.531 |
| 6d$_{5/2}$ | 289.155 | 291.799 | 291.799 |
| 6d$_{3/2}$ | 289.206 | 291.829 | 291.829 |

Table 2. The lifetime (in s) of few low-lying states.

| States | LifeTime |
|--------|----------|
| 3d$_{5/2}$ | 1.274 x 10$^{-7}$ |
| 4s$_{1/2}$ | 7.531 x 10$^{-4}$ |
| 4p$_{1/2}$ | 4.651 x 10$^{-10}$ |
| 4p$_{3/2}$ | 4.563 x 10$^{-10}$ |

Table 3. Oscillator strengths in the length $f_l$ and velocity $f_v$ form for the E1 transitions and its comparison with CIV3 results [15].

| Transitions | $f_l$(CIV3) | $f_l$(CIV3) $f_v$(CC) | $f_v$(CC) |
|-------------|-------------|-----------------------|------------|
| 3d$_{3/2}$ → 4p$_{1/2}$ | 0.0765 | 0.0914 | 0.1588 | 0.1103 |
| 3d$_{3/2}$ → 4p$_{3/2}$ | 0.0154 | 0.0182 | 0.0158 | 0.0109 |
| 3d$_{3/2}$ → 5p$_{1/2}$ | 0.0080 | 0.0091 | 0.0185 | 0.0129 |
| 3d$_{3/2}$ → 5p$_{3/2}$ | 0.0016 | 0.0019 | 0.0037 | 0.0012 |
| 3d$_{3/2}$ → 6p$_{1/2}$ | 0.0030 | 0.0031 | 0.0075 | 0.0042 |
| 3d$_{3/2}$ → 6p$_{3/2}$ | 0.0006 | 0.0007 | 0.0022 | 0.0014 |
| 3d$_{3/2}$ → 4f$_{5/2}$ | 0.1248 | 0.1109 | 0.1020 | 0.1066 |
| 3d$_{3/2}$ → 4f$_{7/2}$ | 0.0925 | 0.1093 | 0.1430 | 0.0982 |
| 3d$_{3/2}$ → 5f$_{5/2}$ | 0.0011 | 0.0111 | 0.0070 | 0.0040 |
| 3d$_{3/2}$ → 6f$_{1/2}$ | 0.0038 | 0.0039 | 0.0076 | 0.0040 |
| 3d$_{3/2}$ → 4f$_{5/2}$ | 0.0600 | 0.0053 | 0.0049 | 0.0041 |
| 3d$_{3/2}$ → 4f$_{7/2}$ | 0.1200 | 0.1069 | 0.1108 | 0.1154 |

Table 4. Transition amplitudes for E2 transitions in length and velocity forms.

| Transitions | Length form | Velocity form |
|-------------|-------------|---------------|
| 3d$_{3/2}$ → 3d$_{3/2}$ | -1.0424 | -1.3694 |
| 3d$_{3/2}$ → 4d$_{3/2}$ | 1.5188 | 1.7331 |
| 3d$_{3/2}$ → 4d$_{3/2}$ | 1.0237 | 0.9783 |
| 3d$_{3/2}$ → 5g$_{7/2}$ | -1.1445 | -1.1284 |
| 3d$_{3/2}$ → 5g$_{7/2}$ | 1.9965 | 2.0618 |
| 3d$_{3/2}$ → 4g$_{9/2}$ | 0.3841 | 0.3787 |
| 3d$_{3/2}$ → 5g$_{7/2}$ | -1.3741 | -1.3381 |
| 3d$_{3/2}$ → 4d$_{3/2}$ | -9.0885 | -8.5152 |
| 3d$_{3/2}$ → 5d$_{3/2}$ | 7.5085 | 9.4869 |
| 3d$_{3/2}$ → 5d$_{3/2}$ | 7.3753 | 7.2191 |
| 3d$_{3/2}$ → 5g$_{7/2}$ | 24.1509 | 24.2467 |
| 3d$_{3/2}$ → 4f$_{5/2}$ | -11.7963 | -11.4311 |
| 3d$_{3/2}$ → 4f$_{5/2}$ | 5.1101 | 5.0902 |
| 3d$_{3/2}$ → 4f$_{5/2}$ | 6.5263 | 6.5279 |
| 3d$_{3/2}$ → 4f$_{5/2}$ | -17.5349 | -18.9716 |

Small that is why it is difficult to comment on this, whatsoever it is worthy to do further study.

Large lifetime has been estimated for the 3d$_{5/2}$ state as seen in table 2 which shows its potentiality as a candidate for plasma temperature diagnostics in stars and plasma fusion devices. The millisecond lived excited 4s state might be important in many astronomical diagnostics.

Table 3 provides the comparison of the CC-calculated electric dipole (E1) oscillator strengths ($f$-value) with the CIV3 [15] results in length and velocity forms. In most of the cases CIV3 underestimate the $f$-values, though there are cases where good agreements are seen among the results obtained.
Table 5. Transition wavelengths, transition amplitudes and transition rates of Ti IV for the electric quadrupole (E2) and magnetic dipole (M1) transitions.

| Transition | $\lambda_{CC}$ | $E_2$ | $M_1$ | $A_{E2}$ | $A_{M1}$ |
|------------|----------------|-------|-------|----------|----------|
| 3d_{3/2} → 3d_{3/2} | -1.0424 | -1.5458 | 2.5881 × 10^{-10} | 7.8411 × 10^{-4} |
| 3d_{3/2} → 4d_{5/2} | 508.81 | 1.5188 | 0.0863 | 1.8939 × 10^{-4} | 1.1808 × 10^{-3} |
| 3d_{3/2} → 4d_{5/2} | 507.48 | 1.0237 | -0.0026 | 5.8116 × 10^{-5} | 2.3251 × 10^{-1} |
| 3d_{3/2} → 5d_{5/2} | 384.18 | 0.5334 | 0.0443 | 9.5185 × 10^{-3} | 2.3338 × 10^{-2} |
| 3d_{3/2} → 5d_{5/2} | 384.12 | 0.3738 | -0.0012 | 3.1188 × 10^{-4} | 1.2934 × 10^{-1} |
| 3d_{3/2} → 6d_{5/2} | 341.62 | 0.3894 | 0.0371 | 9.1246 × 10^{-5} | 2.3281 × 10^{-2} |
| 3d_{3/2} → 6d_{5/2} | 341.57 | 0.2769 | -0.0009 | 3.0781 × 10^{-2} | 9.1375 × 10^{-4} |
| 3d_{3/2} → 4s_{1/2} | 1254.44 | -2.2291 | 8.9573 × 10^{-3} | |
| 3d_{3/2} → 4s_{1/2} | 469.87 | -0.0283 | 1.9581 × 10^{-3} | |
| 3d_{3/2} → 5g_{7/2} | 374.29 | -0.0159 | 1.9271 × 10^{-3} | |
| 3d_{3/2} → 5g_{7/2} | 359.03 | -1.1445 | 3.0738 × 10^{-4} | |
| 3d_{3/2} → 4d_{3/2} | 509.89 | -1.0328 | 0.0012 | 8.6654 × 10^{-3} | 7.3251 × 10^{-2} |
| 3d_{3/2} → 4d_{3/2} | 508.56 | 1.9965 | 0.0241 | 2.1871 × 10^{-4} | 1.9851 × 10^{-1} |
| 3d_{3/2} → 5d_{3/2} | 384.80 | -0.0362 | -0.0009 | 4.2166 × 10^{-5} | 9.5861 × 10^{-1} |
| 3d_{3/2} → 5d_{3/2} | 384.73 | 0.7004 | 0.1239 | 1.0863 × 10^{-2} | 1.2118 × 10^{-3} |
| 3d_{3/2} → 6d_{3/2} | 342.11 | -0.2606 | 0.0008 | 4.0575 × 10^{-4} | 1.0778 × 10^{-1} |
| 3d_{3/2} → 6d_{3/2} | 342.06 | 0.5148 | 0.1035 | 1.0563 × 10^{-4} | 1.2032 × 10^{-3} |
| 3d_{3/2} → 4s_{1/2} | 1261.05 | -2.7489 | 1.3268 × 10^{-3} | |
| 3d_{3/2} → 5s_{1/2} | 470.79 | -0.0467 | 5.2083 × 10^{-4} | |
| 3d_{3/2} → 6s_{1/2} | 374.85 | -0.0229 | 3.9678 × 10^{-3} | |
| 3d_{3/2} → 5g_{7/2} | 359.57 | 0.3841 | 3.4362 × 10^{-4} | |
| 3d_{3/2} → 5g_{7/2} | 359.57 | -1.1741 | 3.5181 × 10^{-4} | |
from both the methods. The good agreement between the results of length and velocity forms indicates the accuracy of the numerical approaches employed.

In table 4, the comparison of the transition amplitudes in length and velocity forms for electric quadrupole ($E2$) transitions among various low-lying excited states is presented. In most of the cases good agreements are seen among the results obtained from both forms, which shows the robustness of numerical approaches employed.

Table 5 presents the $E2$ and $M1$ transition wavelengths, amplitudes and transition rates, respectively, for most of the low-lying states. They are all relevant to astrophysical studies. The calculated wavelengths are in good agreement for most of the cases with the results obtained from the website of NIST [29]. From physics point of view, the important forbidden transitions are the transitions among the fine structures of the 3d and 4p states. Former one falls in the infrared region, which has many applications in the plasma research and infrared laser spectroscopy [30]. The latter one falls in the optical region, which has immense prospect in different atomic physics experiments. We have not reported wavelengths for most of other fine structure transitions those fall far beyond the infrared region.

Table 5. (Continued.)

| Transition | $\lambda_{\infty}$ | $E_J$ | $M_1$ | $A_{E2}$ ($E2$) | $A_{M1}$ ($M1$) |
|------------|--------------------|-------|-------|----------------|-----------------|
| $5g_{7/2} \rightarrow 5g_{9/2}$ | $-21.7248$ | $3.4693 \times 10^{-12}$ |
| $4p_{3/2} \rightarrow 4p_{5/2}$ | $-8.1664$ | $-1.1466$ | $8.0404 \times 10^{-7}$ | $5.3471 \times 10^{-3}$ |
| $3p_{3/2}$ | $967.38$ | $-0.0248$ | $9.1808 \times 10^{-3}$ |
| $5p_{1/2}$ | $964.08$ | $-4.9577$ | $8.2629 \times 10^{3}$ | $1.8068 \times 10^{-1}$ |
| $6p_{1/2}$ | $677.02$ | $-0.0134$ | $7.8039 \times 10^{-1}$ |
| $6p_{3/2}$ | $675.99$ | $-4.4916$ | $4.0016 \times 10^{-4}$ | $1.9647 \times 10^{-1}$ |
| $4p_{5/2}$ | $921.42$ | $-1.7963$ | $3.9106 \times 10^{-4}$ |
| $5f_{1/2}$ | $666.86$ | $3.1836$ | $1.4165 \times 10^{-5}$ |
| $4p_{7/2}$ | $975.35$ | $5.1101$ | $1.6566 \times 10^{-6}$ | $4.8896 \times 10^{-1}$ |
| $5p_{3/2}$ | $972.00$ | $-4.7702$ | $7.3431 \times 10^{-3}$ | $1.7778 \times 10^{-2}$ |
| $6p_{3/2}$ | $680.91$ | $-2.1388$ | $1.7501 \times 10^{-4}$ | $7.1813 \times 10^{-1}$ |
| $6p_{5/2}$ | $679.87$ | $-1.8725$ | $6.7585 \times 10^{-5}$ | $1.5540 \times 10^{-2}$ |
| $4f_{5/2}$ | $928.65$ | $6.3563$ | $1.0919 \times 10^{-4}$ |
| $4f_{7/2}$ | $928.62$ | $-15.5656$ | $4.9119 \times 10^{-4}$ |
| $5f_{5/2}$ | $670.63$ | $-0.8062$ | $8.9437 \times 10^{-4}$ |
| $5f_{7/2}$ | $670.69$ | $2.1849$ | $4.9245 \times 10^{-4}$ |
| $5p_{1/2} \rightarrow 5p_{3/2}$ | $282914.16$ | $-30.1011$ | $1.4052 \times 10^{-7}$ | $3.9431 \times 10^{-4}$ |
| $6p_{1/2} \rightarrow 6p_{3/2}$ | $2255.56$ | $0.0306$ | $1.1004 \times 10$ |
| $6p_{3/2}$ | $2244.24$ | $17.5393$ | $1.4709 \times 10^{3}$ | $7.8445 \times 10^{2}$ |
| $4f_{5/2}$ | $19396.42$ | $-24.4364$ | $4.0591 \times 10^{-2}$ |
| $5f_{5/2}$ | $2146.58$ | $-35.8189$ | $5.2545 \times 10^{-3}$ |
| $5p_{3/2}$ | $2273.69$ | $17.8798$ | $2.9460 \times 10^{2}$ | $9.0885 \times 10^{-2}$ |
| $6p_{3/2}$ | $2262.18$ | $16.7129$ | $1.3201 \times 10^{2}$ | $2.1968 \times 10^{1}$ |
| $4f_{5/2}$ | $20824.11$ | $12.8459$ | $7.8658 \times 10^{-3}$ |
| $4f_{7/2}$ | $20811.39$ | $2.1849$ | $1.7112 \times 10^{4}$ |
| $5f_{5/2}$ | $2177.12$ | $19.3650$ | $1.4311 \times 10^{3}$ |
| $5f_{7/2}$ | $2122.42$ | $47.4574$ | $7.3208 \times 10^{3}$ |
| $6p_{1/2}$ | $6p_{3/2}$ | $-70.0679$ | $-1.1435$ | $7.9082 \times 10^{-6}$ | $9.8773 \times 10^{-5}$ |
| $4f_{5/2}$ | $2552.37$ | $6.9155$ | $8.2409 \times 10^{4}$ |
| $5f_{5/2}$ | $2552.37$ | $6.76077$ | $3.0084 \times 10^{4}$ |
| $6p_{3/2}$ | $2537.88$ | $-3.7780$ | $2.5305 \times 10^{5}$ |
| $4f_{5/2}$ | $2538.11$ | $9.2581$ | $1.1392 \times 10^{6}$ |
| $5f_{5/2}$ | $399.86$ | $-41.2699$ | $3.1101+8$ |
| $5f_{7/2}$ | $399.88$ | $100.9901$ | $1.3964 \times 10^{4}$ |
| $4f_{5/2}$ | $4f_{7/2}$ | $-10.0372$ | $-1.8513$ | $3.0455 \times 10^{-19}$ | $2.9067 \times 10^{-10}$ |
| $5f_{5/2}$ | $2413.71$ | $-14.7715$ | $4.9713 \times 10^{3}$ |
| $5f_{7/2}$ | $2414.52$ | $-6.4105$ | $7.0103 \times 10^{3}$ |
| $4f_{7/2}$ | $2413.71$ | $6.4256$ | $9.0069 \times 10^{3}$ |
| $5f_{7/2}$ | $2414.52$ | $-17.3549$ | $5.1381 \times 10^{3}$ |
| $5f_{5/2}$ | $5f_{7/2}$ | $-35.759$ | $-1.8511$ | $9.6620 \times 10^{-15}$ | $3.1770 \times 10^{-11}$ |
| $4s_{1/2}$ | $4s_{3/2}$ | $751.27$ | $-0.0687$ | $1.5011 \times 10^{2}$ |
| $6s_{1/2}$ | $6s_{3/2}$ | $533.41$ | $-0.0386$ | $1.3240 \times 10^{3}$ |
| $5s_{1/2}$ | $5s_{1/2}$ | $1839.42$ | $0.0837$ | $1.5181 \times 10^{2}$ |
few transitions among the low-lying states. The unusual strong core correlation, almost same as DF, contribution has been found for $E2$ transition among the fine structure of 4p states. Core correlation is the weakest among the three correlations presented in the table. Dominance of pair-correlation effects over the core polarization observed in all the transitions.

Similarly, the quantitative contributions from different correlation terms for few $M1$ transitions among the low-lying states are presented in Table 7. From this table, it is really interesting to see that the low correlation effects, especially core-polarization effects, are almost negligible up to the digits displayed in the table. In few cases, strong pair correlations are noticeable.

| Transition | DF | Core correlation | Pair correlation | Core polarization | Norm | Total |
|------------|--|------------------|------------------|-------------------|------|-------|
| $3d_{5/2} \rightarrow 3d_{5/2}$ | $-1.1938$ | $0.0010$ | $0.0688$ | $0.0794$ | $0.0223$ | $-1.0424$ |
| $3d_{3/2} \rightarrow 3d_{3/2}$ | $1.5863$ | $-0.0016$ | $-0.1227$ | $0.0198$ | $-0.0234$ | $1.5188$ |
| $3d_{3/2} \rightarrow 4d_{3/2}$ | $1.0364$ | $-0.0003$ | $-0.0477$ | $0.0385$ | $-0.0160$ | $1.0237$ |
| $3d_{5/2} \rightarrow 5d_{5/2}$ | $0.5426$ | $0.0025$ | $-0.0469$ | $0.0341$ | $-0.0328$ | $-2.1843$ |
| $3d_{3/2} \rightarrow 4s_{1/2}$ | $-2.3347$ | $0.0050$ | $0.1626$ | $-0.0269$ | $0.0328$ | $-2.2291$ |
| $3d_{5/2} \rightarrow 5s_{1/2}$ | $-0.0597$ | $0.0009$ | $0.0076$ | $0.0093$ | $0.0004$ | $-0.0263$ |
| $3d_{3/2} \rightarrow 4d_{5/2}$ | $-1.0433$ | $0.0001$ | $0.0464$ | $-0.2254$ | $0.0157$ | $-1.0322$ |
| $3d_{5/2} \rightarrow 4d_{5/2}$ | $2.0825$ | $-0.0001$ | $-0.1589$ | $0.0726$ | $0.3562$ | $1.9965$ |
| $3d_{5/2} \rightarrow 4s_{1/2}$ | $-2.8689$ | $0.0076$ | $0.1983$ | $-0.0125$ | $-0.0401$ | $-2.7489$ |
| $4d_{5/2} \rightarrow 5d_{5/2}$ | $-5.1218$ | $0.0071$ | $0.0922$ | $-0.0167$ | $0.0511$ | $-5.3540$ |
| $4d_{3/2} \rightarrow 5d_{3/2}$ | $10.9993$ | $-0.0046$ | $-1.0611$ | $0.0319$ | $-0.0978$ | $9.0113$ |
| $5d_{5/2} \rightarrow 4s_{1/2}$ | $0.9699$ | $-0.0051$ | $-0.2398$ | $-0.0268$ | $-0.0066$ | $0.7484$ |
| $5d_{5/2} \rightarrow 5s_{1/2}$ | $-25.758$ | $0.0538$ | $0.5885$ | $0.0133$ | $0.1695$ | $-24.9925$ |
| $5d_{5/2} \rightarrow 5s_{1/2}$ | $-0.0753$ | $-0.0014$ | $0.0072$ | $-0.0786$ | $0.0006$ | $0.0467$ |
| $4p_{1/2} \rightarrow 4p_{1/2}$ | $-8.6289$ | $-0.0251$ | $0.5297$ | $0.0812$ | $0.1789$ | $-8.1664$ |
| $5p_{1/2} \rightarrow 4p_{1/2}$ | $-5.2202$ | $0.0137$ | $-0.1654$ | $-0.0293$ | $0.0335$ | $-5.1101$ |
| $5p_{1/2} \rightarrow 5p_{1/2}$ | $-31.4436$ | $0.1799$ | $1.0952$ | $0.0301$ | $0.0888$ | $-30.1611$ |

Table 7. Explicit contributions from the MR-FSCCSD(T) calculations to the absolute magnitude of the reduced $M1$ transition matrix elements in au.

| Transition | DF | Core correlation | Pair correlation | Core polarization | Norm | Total |
|------------|--|------------------|------------------|-------------------|------|-------|
| $3d_{5/2} \rightarrow 3d_{5/2}$ | $-1.5489$ | $0.0005$ | $0.0000$ | $0.0000$ | $0.0333$ | $-1.5458$ |
| $3d_{3/2} \rightarrow 4d_{3/2}$ | $-0.0015$ | $-0.0000$ | $0.0097$ | $0.0001$ | $0.0000$ | $-0.0026$ |
| $3d_{5/2} \rightarrow 4d_{5/2}$ | $-0.0017$ | $0.0001$ | $-0.0099$ | $-0.0002$ | $0.0000$ | $-0.0012$ |
| $3d_{3/2} \rightarrow 4d_{5/2}$ | $-0.0007$ | $0.0001$ | $0.1857$ | $-0.0000$ | $-0.0038$ | $0.2407$ |
| $3d_{5/2} \rightarrow 5d_{3/2}$ | $-0.0001$ | $-0.0001$ | $-0.0061$ | $-0.0001$ | $-0.0000$ | $-0.0008$ |
| $4d_{3/2} \rightarrow 4d_{3/2}$ | $-1.5491$ | $0.0003$ | $0.0000$ | $0.0000$ | $0.0153$ | $-1.5485$ |
| $5d_{3/2} \rightarrow 5d_{3/2}$ | $-1.5492$ | $0.0019$ | $0.0001$ | $0.0000$ | $0.0147$ | $-1.5479$ |
| $4p_{1/2} \rightarrow 5s_{1/2}$ | $0.0004$ | $-0.0006$ | $0.0560$ | $0.0000$ | $0.0004$ | $0.0687$ |
| $4p_{1/2} \rightarrow 4p_{1/2}$ | $-1.1545$ | $0.0059$ | $0.0000$ | $0.0000$ | $0.0125$ | $-1.1466$ |
| $4p_{1/2} \rightarrow 5p_{1/2}$ | $0.0000$ | $0.0000$ | $-0.0207$ | $0.0000$ | $0.0002$ | $-0.0248$ |
| $4p_{1/2} \rightarrow 5p_{1/2}$ | $-0.0059$ | $0.0108$ | $-0.0060$ | $0.0000$ | $-0.0000$ | $0.0049$ |

In this paper, we have reported the excitation energies for a few excited states of Ti IV by using the MR-FSCCSD(T) method, which are in excellent agreement with the NIST results. Magnetic dipole and electric quadrupole transition amplitudes among the bound states of the system are important for the astronomical observations and plasma researches. Here, we have reported these results for the first time. Especially, the forbidden transitions between the fine structure 4p states may be considered for different atomic experiments of fundamental physics due to its optical transition line. Long lifetime has been observed for the first excited 3d$_{5/2}$ state and it can be used as potential metastable state for experimental physics. We have also highlighted different correlation effects arising through the MR-FSCCSD(T) method.

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