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

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(Dated: February 1, 2008)

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-art all-order many-body theory called Coupled Cluster (CC) theory in the relativistic frame-work. 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 very good agreement with the measurements. Also we compare our calculated electric dipole (E1) transition amplitudes of few transitions with recent many-body calculations by different groups. We have also carried out the calculations for the lifetimes of the low-lying states of Ti IV. A long lifetime is found for the first excited $3d^2D_{5/2}$ state, which suggested that Ti IV may be one of the useful candidates for many important studies. Most of the results reported here are not available in the literature, to the best of our knowledge.

I. INTRODUCTION

With the advent of improved technologies in both observational instruments in astronomy and laboratory instruments in plasma and atomic research, accurate transitions rates ve been possible in high resolution spectrums. However, in many of the cases, especially for forbidden transitions of stripped electronic systems experimental measurements are difficult. Whereas, those transitions are very important in various fields of science and technology. Therefore, there are urgent requirement for accurate theoretical estimations for these transitions rates to meet the demands. The forbidden lines provide important clues in other areas of astrophysics, beacuse of the long lifetime of the upper state against radiative decay. These lines are particularly sensitive to the

collisional de-excitation and serve as indicators of electron density and temparature, N_e and T_e, in the emmision region. Determination of N_e and T_e from the forbidden line intensities was discussed origanally for the general case by Seaton [1] and Seaton and Osterbrock [2]. A number of such transitions have been observed in the ultraviolet spectrum of the solar corona. Forbidden atomic emmision lines are commonly observed in quasars with an intensity often comparable to accompanying 'allowed transition' [3]. Moreover, gaseous nebulae exhibit in their spectra forbidden transition lines of low excitation energy. Many astrophysical phenomena like coronal heating, evolution of chemical composition in stellar envelopes, determination of the chemistry in the planetary nebulae precursor's envelope are believed to be explained largely by these forbidden lines. In laboratory tokamak plasmas and in various astronomical objects, suitably chosen these forbidden lines serve as a basis for reliable electron density and temperature diagnostics [4]. Titanium is observed in a variety of stellar objects, like in the Sun where Ti figures in third place in terms of number of lines [5]. Various ionization stages of Ti are present in stellar plasma, for instance in the τ Sco spectrum [6]. Recently, the lines of triply ionized titanium (Ti IV) have been detected in Wolf-Rayet Star [7]. Also, Ti IV in oxidized form used in dark and photo induced decomposition of ozone in air has been studied [8]. Accurate estimation of forbidden transitions of this ionized system are urgent to explain and quantify the band structure of the energy level of this system doped in crystal material. Doping of Ti IV in crystal material is used to build optical and polymer devices [9].

In this work, we employ the multi-reference (MR) Fock-space Coupled Cluster (FSCC) method with single (S), double (D) and partial triple (T) excitation to compute forbidden transitions in Ti IV using relativistic orbitals/ spinors. The coupled-cluster (CC) theory is non-perturbative in nature and its relativistic extension has been successfully employed earlier in many sophisticated problems [10, 11] to estimate various tiny effects precisely. In the present work, we investigate the core and valence electrons correlation contributions obtained from the MR-FSCCSD(T) method to the M1 and E2 transitions among the low-lying states in the considered system.

Because of its complexity and computational limitations, we have considered only the single, double and partially triple excitations in the CC theory. However, due to its all-orderness and also because the contributions from higher order excitations diminishes gradually, this is a quite accurate calculation. Some of the detail applications in astrophysics and scattering physics of Ti IV are discussed in recent paper by Kingston and Hibbert [12]. They have used non-relativistic configuration interaction method for electromagnetically allowed transitions and considered relativistic effect with Breit-Pauli approximation. Length and velocity forms of the transition amplitudes are

compared for few allowed transitions to check the accuracy of the numerical approaches used.

II. THEORY

Coupled Cluster (CC) theory for one electron attachment process

The CC theory in the relativistic framework can be extended open-shell theory based on the no-virtual-pair approximation (NVPA) along with appropriate modification of orbital form and potential terms [13]. Relativistic CC theory begins with Dirac-Coulomb Hamiltonian (H) for an N electron atom. The Fock-space multireference CC (FSMRCC) approach used for any valence orbitals is employed here.

Since the FSMRCC theory has been described elsewhere [14, 15, 16, 17], we provide a brief review of this method. The FSMRCC theory for single valence orbital is based on the concept of the common vacuum for both the N and N+1 electron systems, which allows us to formulate a direct method of excitation energies. In this method the holes and particles are defined with respect to the common vacuum for both the N and N+1 electron systems. The model space of a (m,n) Fock-space contains determinants with m holes and n particles distributed within a set of what are termed as *active* orbitals. For example, in this present paper, we are dealing with a (0,1) Fock space, which is a complete model space (CMS) by construction and is given by

$$|\Psi_\mu^{(0,1)}\rangle = \sum_i \mathrm{C}_{i\mu}|\Phi_i^{(0,1)}\rangle, \tag{2.1}$$

where $\mathrm{C}_{i\mu}$'s are the coefficients of $\Psi_\mu^{(0,1)}$ and $\Phi_i^{(0,1)}$'s are the model space configurations. The dynamical electron correlation effects are introduced through the *valence-universal* wave-operator Ω [15, 18]

$$\Omega = \{\exp(\tilde{S})\}, \tag{2.2}$$

where

$$\tilde{S} = \sum_{k=0}^{m}\sum_{l=0}^{n} S^{(k,l)} = S^{(0,0)} + S^{(0,1)} + S^{(1,0)} + \cdots. \tag{2.3}$$

Here $\{\cdots\}$ stands for the normal odering of the creation and annihilation operators related with corresponding excitations operators, S. For example, the normal ordered form of the Dirac-Coulomb

Hamiltonian used here is given by

$$\mathcal{H} = \mathrm{H} - \langle\Phi|\mathrm{H}|\Phi\rangle = \mathrm{H} - \mathrm{E_{DF}} = \sum_{ij}\langle i|f|j\rangle\left\{a_i^\dagger a_j\right\} + \frac{1}{4}\sum_{i,j,k,l}\langle ij||kl\rangle\left\{a_i^\dagger a_j^\dagger a_l a_k\right\}, \tag{2.4}$$

where

$$\langle ij||kl\rangle = \langle ij|\frac{1}{r_{12}}|kl\rangle - \langle ij|\frac{1}{r_{12}}|lk\rangle. \tag{2.5}$$

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

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

$$\Omega = exp(T)\{\exp(S_v)\}. \tag{2.6}$$

Now, if we define

$$\mathrm{H_{eff}} = \mathrm{P^{(k,l)}H\Omega_v P^{(k,l)}}. \tag{2.7}$$

with the operator $P^{(\mathrm{k,l})}$ is the model space projector for k-hole and l-particle, which satisfying complete model space condition. The "valence-universal" wave-operator Ω in Eq.(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

$$\mathrm{H\Omega P^{(k,l)}} = \mathrm{\Omega P^{(k,l)}.H_{eff}P^{(k,l)}} \tag{2.8}$$

To formulate the theory for direct energy differences, we pre-multiply Eq.(2.8) by e^{-T} and get

$$\mathrm{\overline{H}\Omega_v P^{(k,l)}} = \mathrm{\Omega_v P^{(k,l)}H_{eff}P^{(k,l)}} \quad \forall(k,l) \neq (0,0), \tag{2.9}$$

where $\overline{\mathrm{H}}$=e^{-T} H e^{T}. Since $\overline{\mathrm{H}}$ can be partitioned into a connected operator $\tilde{\mathrm{H}}$ and $\mathrm{E_{ref/gr}}$ (N-electron closed-shell reference or ground state energy), we likewise define $\tilde{\mathrm{H}}_{\mathrm{eff}}$ as

$$\mathrm{H_{eff}} = \tilde{\mathrm{H}}_{\mathrm{eff}} + \mathrm{E_{ref/gr}}. \tag{2.10}$$

Substituting Eq. (2.10) in Eq. (2.9) we obtain the Fock-space Bloch equation for energy differences:

$$\mathrm{\tilde{H}\Omega_v P^{(k,l)}} = \mathrm{\Omega_v P^{(k,l)}\tilde{H}_{eff}P^{(k,l)}}. \tag{2.11}$$

Eqs. (2.8) and (2.11) are solved by Bloch projection method, involving the left projection of the equation with $\mathrm{P}^{(\mathrm{k,l})}$ and its orthogonal complement $\mathrm{Q}^{(\mathrm{k,l})}$ to obtain the effective Hamiltonian and the cluster amplitudes, respectively.

In this article, triple excitations are included in the open shell CC amplitude which correspond to the correlation to the valence orbitals, by an approximation that is similar in spirit to CCSD(T) [19]. The approximate valence triple excitation amplitude is given by

$$S^{(0,1)}{}^{pqr}_{abk} = \frac{\{\widehat{VT_2}\}^{pqr}_{abk} + \{\widehat{VS^{(0,1)}{}_2}\}^{pqr}_{abk}}{\varepsilon_a + \varepsilon_b + \varepsilon_k - \varepsilon_p - \varepsilon_q - \varepsilon_r}, \tag{2.12}$$

where $S^{(0,1)}{}^{pqr}_{abk}$ are the amplitudes corresponding to the simultaneous excitation of orbitals a, b, k to p, q, r, respectively; $\widehat{VT_2}$ and $\widehat{V\mathrm{S}^{(0,1)}{}_2}$ are the connected composites involving V and T, and V and $S^{(0,1)}$, respectively, where V is the two electron Coulomb integral and ε's are the orbital energies.

III. COMPUTATIONAL PROCEDURE

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

$$\begin{aligned} D_{fi} &= \frac{\langle\Psi_f|D|\Psi_i\rangle}{\sqrt{\langle\Psi_f|\Psi_f\rangle\langle\Psi_i|\Psi_i\rangle}} \\ &= \frac{\langle\Phi_f|\{1+S_f^{(0,1)^\dagger}\}e^{T^\dagger}De^T\{1+S_i^{(0,1)}\}|\Phi_i\rangle}{\sqrt{\langle\Phi_f|\{1+S_f^{(0,1)^\dagger}\}e^{T^\dagger}e^T\{1+S_f^{(0,1)}\}|\Phi_f\rangle\langle\Phi_i|\{1+S_i^{(0,1)^\dagger}\}e^{T^\dagger}e^T\{1+S_i^{(0,1)}\}|\Phi_i\rangle}}. \end{aligned} \tag{3.1}$$

Here, only consideraion comes from single power of the $S^{(0,1)}$ operator with $S_1^{(0,1)}$ and $S_2^{(0,1)}$ representing single excitation operators from valence orbital and double excitations from core-valence orbitals, respectively. Interesting correlation features of the transition operator D are found in the contraction of $\overline{D}$ with $S_1^{(0,1)}$ and $S_2^{(0,1)}$, which represent 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 this CCSD(T) calculation.

For computational simplicity, we express $\overline{D}$ as effective terms using the generalized Wick's theorem [14] as

$$\overline{D} = (e^{T^\dagger}De^T)_{f.c.} + (e^{T^\dagger}De^T)_{o.b.} + (e^{T^\dagger}De^T)_{t.b.} + ..., \tag{3.2}$$

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 $\overline{D}$, the effective one-body and two-body terms are computed keeping terms of the form of

$$\overline{D}_{o.b.} = D + T^{\dagger}D + DT + T^{\dagger}DT, \tag{3.3}$$

and

$$\overline{D}_{t.b.} = DT_1 + T_1^{\dagger}D + DT_2 + T_2^{\dagger}D, \tag{3.4}$$

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 element corresponding to E1, E2 and M1 transitions are given earlier papers written by few of the authors [20, 21]. The emission transition probabilities (in $sec^{(-1)}$) for the E1, E2 and M1 channels from states f to i are given by

$$A^{E1}_{f\rightarrow i} = \frac{2.0261 \times 10^{18}}{\lambda^3 [j_f]} S^{E1}_{f\rightarrow i} \tag{3.5}$$

$$A^{E2}_{f\rightarrow i} = \frac{1.11995 \times 10^{18}}{\lambda^5 [j_f]} S^{E2} \tag{3.6}$$

$$A^{M1}_{f\rightarrow i} = \frac{2.69735 \times 10^{13}}{\lambda^3 [j_f]} S^{M1}, \tag{3.7}$$

where $[j_f] = 2j_f + 1$ 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 λ (in Å) are the corresponding transition wavelength.

IV. RESULT AND DISCUSSIONS

Many-body calculations started with closed shell coupled cluster calculations of Ti V. The reference state of this closed shell system is obtained from Dirac-Fock (DF) calculation using Gaussian type orbital (GTO) formalism [22]. The exponent of the GTO functions are obtained from universal even temporing condition with $\alpha = 0.00825$ and $\beta = 2.73$ for all the symmetries. The number basis function 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

TABLE I: Ionisation Potential(IP) in cm^{-1} of different levels of Ti IV and its comparison with NIST value and MCHF values and the Fine Structure Splitting(FSS)

	IP			FSS		
States	NIST	MCHF	CC	NIST	MCHF	CC
$3d_{3/2}$	0	0	0			
$3d_{5/2}$	382.10	790.11	418.02	382.10	790.11	418.02
$4s_{1/2}$	80388.92		79716.67			
$4p_{1/2}$	127921.36	124749.38	127689.51			
$4p_{3/2}$	128739.59	125539.49	128534.43	818.23	790.10	844.91
$4d_{5/2}$	196889.96		197050.03	85.69		96.80
$5s_{1/2}$	212407.34		212823.15			
$5p_{1/2}$	230608.89	228714.51	231061.48	315.49	263.37	353.46
$5p_{3/2}$	230924.38	228977.88	231414.94			
$4f_{5/2}$	236135.29	234881.75	236217.07			
$4f_{7/2}$	236142.30	235254.86	236220.0	7.01	373.10	3.71
$5d_{3/2}$	258838.48		260290.41			
$5d_{5/2}$	258877.08		260335.26	38.94		44.85
$6s_{1/2}$	265847.42		267187.94			
$6p_{1/2}$	274726.29	272719.18	275396.29			
$6p_{3/2}$	274881.21	272828.92	275620.04	154.92	109.74	223.75
$5f_{5/2}$	275847.01	276669.72	277647.10			
$5f_{7/2}$	275861.94	277942.67	277633.09	14.93	1272.95	14.01
$5g_{7/2}$	278510.63		278530.47			
$5g_{9/2}$	278511.23		278531.05	0.60		0.58
$6d_{3/2}$	289185.99		292720.83			
$6d_{5/2}$	289206.93		292760.30	20.94		60.30

this calculations are based on convergent criteria of core correlation energy for which it satisfies numerical completeness.

In Table I, we have shown the ionisation potential obtained using the CCSD(T) method of a few low-lying excited states taking $3d_{3/2}$ as a ground state. Kingston and Hibbert [12] have also calculated few of them by multiconfiguration Hartree-Fock (MCHF) method. Our calculated results are in better agreement with the experiemnetal results (obtained from NIST [23]) in comparision with the MCHF results. Except for $3d_{5/2}$ state, the average deviation with the NIST results is

only 0.427%, whereas in the MCHF method it is 1.08%. The CC calculated fine structure splitting (FS) of $3d$ has far better agreement than MCHF calculation. Also, the excellent agreement of the FS splittings of F states indicates the accurate description of correlation in the CC approach. Especially, the all order considerations of core-polarization and pair-correlations.

Large lifetime has been estimated for $3d_{5/2}$ state as seen in table II shows its potentiality as a candidate for plasma temperature disgonistics in stars and plasma fusion devices. The millisecond lived excited state $4s$ might have importance in many astronomical diagonistics.

TABLE II: The lifetime(in Sec) of few low-lying states

States	Lifetime
$3d_{5/2}$	1.274E+03
$4s_{1/2}$	7.531E-04
$4p_{1/2}$	4.651E-10
$4p_{3/2}$	4.563E-10

Table III provides the comparison of the CC calculated electric dipole (E1) oscillator strengths (f-value) with the MCHF [12] in length and velocity form. In most of the cases MCHF underestimate the f-values, though there are cases where good agreement seen among the results obtained from both the methods. The good agreement between the results of length and velocity forms indicates the accuracy of the numerical approaches employed.

Table IV presents the electric quadrupole and magnetic dipole transition wavelengths and amplitudes, respectively, for most of the low-lying states. They are all relevant to astrophysically studies. The calculated wavelengths have good agreement for most of the cases with the result obtained from the website of National Institute of Standard and Technology (NIST) [23]. From physics point of view, the important transitions among these are the forbidden 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 [24]. The latter one falls in the optical region, 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.

Quantitative contributions from different correlation terms for few E2 transitions among low-lying states are presented in Table V. The table shows a comparative estimations of core-

TABLE III: Oscillator strengths in the length f_l and velocity f_v form for E_1 transitions and its comparison with MCHF results[12].

Transitions		f_l(MCHF)	f_v(MCHF)	f_l(CC)	f_v(CC)
$3d_{3/2}$	$\rightarrow 4p_{1/2}$	0.0765	0.0914	0.1588	0.1103
	$\rightarrow 4p_{3/2}$	0.0154	0.0182	0.0158	0.0109
	$\rightarrow 5p_{1/2}$	0.0080	0.0091	0.0185	0.0129
	$\rightarrow 5p_{3/2}$	0.0016	0.0019	0.0037	0.0012
	$\rightarrow 6p_{1/2}$	0.0030	0.0031	0.0075	0.0042
	$\rightarrow 6p_{3/2}$	0.0006	0.0007	0.0022	0.0014
	$\rightarrow 4f_{5/2}$	0.1248	0.1109	0.1020	0.1066
$3d_{5/2}$	$\rightarrow 4p_{3/2}$	0.0925	0.1093	0.1430	0.0982
	$\rightarrow 5p_{3/2}$	0.0011	0.0111	0.0017	0.0112
	$\rightarrow 6p_{3/2}$	0.0038	0.0039	0.0076	0.0040
	$\rightarrow 4f_{5/2}$	0.0060	0.0053	0.0049	0.0041
	$\rightarrow 4f_{7/2}$	0.1200	0.1069	0.1108	0.1154

polarization, core-correlation and pair-correlation effects in these transitions. The diagrams involving these contributions are discussed in our earlier papers [25]. Though all order effect of core-polarization and pair correlation contributions are considered in the calculations here. Table shows the lowest order contributions of them for few transitions among the low-lying states. The unusual strong core correlation, almost same as DF, contribution has been seen for E2 transition among the fine structure states of $4p$. Core correlation are weakest among the three correlations presented in the table. Dominance of pair correlation effects over core polarization observed in all the transitions.

In ths similar manner the Quantitative contributions from different correlation terms for few M1 transitions among low-lying states are presented in Table VI. From the table VI, it is really interesting to see low correlation effects, especially, core porization effect is almost negigible up to the digits displayed in the table. Few cases, strong pair correlations are noticeable.

V. CONCLUSION

In this paper, we have reported the ionisation potential of a few excited states of Ti IV by using the MR-FSCCSD(T) method, which are in excillent with the NIST results. Magnetic dipole and electric quadrupole transition amplitudes among the bound states of the system are important for

astronomical observations and plasma researches. Here, we have reported these results for the first time. Especially, 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 D- state and it can be used as potential metastable state for experiments in physics. We have also highlighted different correlation effects arising through the MR-FSCCSD(T) method.

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TABLE IV: Transition wavelengths and transition amplitudes of Ti IV for electric quadrupole (E2) and magnetic dipole transitions (M1)

Transition		λ_{CC}	E_2	M_1
$3d_{3/2}$	$\rightarrow 3d_{5/2}$		-1.0336	-1.5458
	$\rightarrow 4d_{3/2}$	508.81	1.4928	0.0863
	$\rightarrow 4d_{5/2}$	507.48	1.0186	-0.0026
	$\rightarrow 5d_{3/2}$	384.18	0.5334	0.0443
	$\rightarrow 5d_{5/2}$	384.12	0.3738	-0.0012
	$\rightarrow 6d_{3/2}$	341.62	0.3894	0.0371
	$\rightarrow 6d_{5/2}$		0.2769	-0.0009
	$\rightarrow 4s_{1/2}$	1254.44	-2.1842	
	$\rightarrow 5s_{1/2}$	469.87	-0.0283	
	$\rightarrow 6s_{1/2}$	374.29	-0.0159	
	$\rightarrow 5g_{7/2}$	359.03	-1.1243	
$3d_{5/2}$	$\rightarrow 4d_{3/2}$	509.89	-1.0034	0.0012
	$\rightarrow 4d_{5/2}$	508.56	1.9701	0.0241
	$\rightarrow 5d_{3/2}$	384.80	-0.3562	-0.0009
	$\rightarrow 6d_{3/2}$	342.11	-0.2606	0.0008
	$\rightarrow 4s_{1/2}$	1261.05	-2.6593	
	$\rightarrow 5s_{1/2}$	470.79	-0.0467	
	$\rightarrow 6s_{1/2}$	374.85	-0.0229	
	$\rightarrow 5g_{7/2}$	359.57	0.3775	
	$\rightarrow 5g_{9/2}$	359.57	-1.3342	
	$\rightarrow 6d_{5/2}$			0.1035
	$\rightarrow 5d_{5/2}$	384.73		0.1239
$4d_{3/2}$	$\rightarrow 4d_{5/2}$		-9.1095	-1.5485
	$\rightarrow 5d_{3/2}$	1568.49	7.4885	0.1370
	$\rightarrow 5d_{5/2}$	1567.39	5.3203	-0.0010
	$\rightarrow 6d_{3/2}$	1039.66	2.3737	-0.0010
	$\rightarrow 6d_{5/2}$		1.8081	-0.0004
	$\rightarrow 4s_{1/2}$	856.02	7.3600	
	$\rightarrow 5s_{1/2}$	6139.37	14.7325	
	$\rightarrow 6s_{1/2}$	1415.37	-2.0579	
	$\rightarrow 5g_{7/2}$	1219.58	24.1136	

(Continuation of Table IV)

Transition		λ_{CC}	E_2	M_1
$4d_{5/2}$	$\rightarrow 5d_{3/2}$	1568.49	-5.3540	-0.0022
	$\rightarrow 5d_{5/2}$	1567.39	9.8113	0.3836
	$\rightarrow 6d_{3/2}$	1039.66	-1.8214	–0.0015
	$\rightarrow 6d_{5/2}$	6139.51	3.0965	0.2316
	$\rightarrow 4s_{1/2}$	856.03	8.9919	
	$\rightarrow 5s_{1/2}$	6139.51	18.0734	
	$\rightarrow 6s_{1/2}$	1413.37	-2.5365	
	$\rightarrow 5g_{7/2}$	1219.57	-8.0497	
	$\rightarrow 5g_{9/2}$	1219.57	28.4611	
$5d_{5/2}$	$\rightarrow 6d_{3/2}$	3087.79	-15.4604	-0.0021
	$\rightarrow 6d_{5/2}$			0.5057
	$\rightarrow 4s_{1/2}$	553.65	0.9166	
	$\rightarrow 5s_{1/2}$	2104.73	-30.6035	
	$\rightarrow 6s_{1/2}$	14592.83	58.9756	
	$\rightarrow 5g_{7/2}$	5495.95	24.2502	
	$\rightarrow 5g_{9/2}$	5495.77	-85.7563	
$5d_{3/2}$	$\rightarrow 5d_{5/2}$		-33.0491	-1.5479
	$\rightarrow 6d_{3/2}$	3083.52	28.4053	0.1803
	$\rightarrow 6d_{5/2}$		15.3297	-0.0019
	$\rightarrow 4s_{1/2}$	533.79	0.7484	
	$\rightarrow 5s_{1/2}$	2106.73	-24.9925	
	$\rightarrow 6s_{1/2}$	14497.95	48.0724	
	$\rightarrow 5g_{7/2}$	5482.44	-72.6985	
$6d_{3/2}$	$\rightarrow 4s_{1/2}$	469.47	0.5346	
	$\rightarrow 5s_{1/2}$	1251.60	-6.2888	
	$\rightarrow 6s_{1/2}$	3916.52	-60.8104	
	$\rightarrow 5g_{7/2}$	6627.89	42.6236	
$6d_{5/2}$	$\rightarrow 4s_{1/2}$	469.38	0.6626	
	$\rightarrow 5s_{1/2}$	1250.98	-7.7575	
	$\rightarrow 6s_{1/2}$	3910.47	-74.4313	
	$\rightarrow 5g_{5/2}$	7027.49	-14.1738	
	$\rightarrow 5g_{9/2}$	7027.77	50.1131	
$5g_{7/2}$	$\rightarrow 5g_{9/2}$		-21.7443	
$4p_{1/2}$	$\rightarrow 4p_{3/2}$		-16.4408	-1.1466
	$\rightarrow 5p_{1/2}$	967.38		-0.0248
	$\rightarrow 5p_{3/2}$	964.08	-10.2894	0.0049
	$\rightarrow 6p_{1/2}$	677.02		-0.0134
	$\rightarrow 6p_{3/2}$	675.99		0.0030
	$\rightarrow 4f_{5/2}$	921.42	24.9090	

(Continuation of Table IV)

Transition		λ_{CC}	E_2	M_1
$4p_{3/2}$	$\rightarrow 5p_{1/2}$	975.35	-5.3367	0.0058
	$\rightarrow 5p_{3/2}$	972.00	-4.7702	-0.1556
	$\rightarrow 6p_{1/2}$	680.91	-2.1388	0.0041
	$\rightarrow 6p_{3/2}$	679.87	-1.8725	-0.0851
	$\rightarrow 4f_{5/2}$	928.65	6.3548	
	$\rightarrow 4f_{7/2}$	928.62	-15.5754	
	$\rightarrow 5f_{5/2}$	670.63	-0.8062	
	$\rightarrow 5f_{7/2}$	670.69	2.1849	
$5p_{1/2}$	$\rightarrow 5p_{3/2}$	282914.16	-30.1611	-1.1508
	$\rightarrow 6p_{1/2}$	2255.56		0.0306
	$\rightarrow 6p_{3/2}$	2244.24	17.5393	-1.1467
	$\rightarrow 4f_{5/2}$	19396.42	-24.4364	
	$\rightarrow 5f_{5/2}$	2146.58	-35.8189	
$5p_{3/2}$	$\rightarrow 6p_{1/2}$	2273.69	17.8798	-0.0089
	$\rightarrow 6p_{3/2}$	2262.18	16.7129	0.1942
	$\rightarrow 4f_{5/2}$	20824.11	12.8459	
	$\rightarrow 4f_{7/2}$	20811.39	2.1849	
	$\rightarrow 5f_{5/2}$	2177.12	19.3650	
	$\rightarrow 5f_{7/2}$	2122.42	47.4574	
$6p_{1/2}$	$\rightarrow 6p_{3/2}$		-70.9679	-1.1435
	$\rightarrow 4f_{5/2}$	2552.37	6.9155	
	$\rightarrow 5f_{5/2}$		76.6077	
$6p_{3/2}$	$\rightarrow 4f_{5/2}$	2537.88	-3.7780	
	$\rightarrow 4f_{7/2}$	2538.11	9.2581	
	$\rightarrow 5f_{5/2}$	399.86	-41.2699	
	$\rightarrow 5f_{7/2}$	399.88	100.9901	
$4f_{5/2}$	$\rightarrow 4f_{7/2}$		-10.0372	-1.8513
	$\rightarrow 5f_{5/2}$	2413.71	-14.7715	
	$\rightarrow 5f_{7/2}$	2414.52	-6.4105	
$4f_{7/2}$	$\rightarrow 5f_{5/2}$	2413.71	6.4049	
	$\rightarrow 5f_{7/2}$	2414.52	-17.4159	
$5f_{5/2}$	$\rightarrow 5f_{7/2}$		-35.759	-1.8511
$4s_{1/2}$	$\rightarrow 5s_{1/2}$	751.27		-0.0687
	$\rightarrow 6s_{1/2}$	533.41		-0.0386
$5s_{1/2}$	$\rightarrow 6s_{1/2}$	1839.42		0.0837

TABLE V: Explicit contributions from the MR-FSCCSD(T) calculations to the absolute magnitude of reduced E2 transitions matrix elements in a.u.

Transition	DF	$Core-Correlation$	$Pair-Correlation$	$Core-Polarization$	$Norm$	$Total$
$3d_{3/2} \rightarrow 3d_{5/2}$	-1.1938	0.0010	0.0688	0.0794	0.0223	-1.0335
$3d_{3/2} \rightarrow 4d_{3/2}$	1.5863	-0.0016	-0.1227	0.0198	-0.0234	1.4928
$3d_{3/2} \rightarrow 4d_{5/2}$	1.0364	-0.0003	-0.0477	0.0385	-0.0160	1.0186
$3d_{3/2} \rightarrow 5d_{3/2}$	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	-2.1843
$3d_{3/2} \rightarrow 5s_{1/2}$	-0.0597	0.0009	0.0076	0.0093	0.0004	-0.0283
$3d_{5/2} \rightarrow 4d_{3/2}$	-1.0433	0.0001	0.0464	-0.2254	0.0157	-1.0003
$3d_{5/2} \rightarrow 4d_{5/2}$	2.0825	-0.0001	-0.1589	0.0726	0.3562	1.9701
$3d_{5/2} \rightarrow 4s_{1/2}$	-2.8689	0.0076	0.1983	-0.0125	-0.0401	-2.6593
$4d_{5/2} \rightarrow 5d_{3/2}$	-5.5128	0.0071	0.0922	-0.0167	0.0511	-5.3540
$4d_{5/2} \rightarrow 5d_{5/2}$	10.9993	-0.0046	-1.0611	0.0319	-0.0978	9.0113
$5d_{3/2} \rightarrow 4s_{1/2}$	0.9699	-0.0051	-0.2398	-0.0268	-0.0066	0.7484
$5d_{3/2} \rightarrow 5s_{1/2}$	-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
$4p_{1/2} \rightarrow 4p_{3/2}$	-8.6289	-8.5459	0.5297	0.0812	0.1789	-16.4408
$5p_{1/2} \rightarrow 4p_{3/2}$	-5.2202	0.0137	-0.1654	-0.0293	0.0335	-5.3369
$5p_{1/2} \rightarrow 5p_{3/2}$	-31.4436	0.1799	1.0952	0.0301	0.0888	-30.1611

TABLE VI: Explicit contributions from the MR-FSCCSD(T) calculations to the absolute magnitude of reduced M1 transitions matrix elements in a.u.

Transition	DF	$Core-Correlation$	$Pair-Correlation$	$Core-Polarization$	$Norm$	$Total$
$3d_{3/2} \rightarrow 3d_{5/2}$	-1.5489	0.0005	0.0000	0.0000	0.0333	-1.5458
$3d_{3/2} \rightarrow 4d_{5/2}$	-0.0015	-0.0000	0.0097	0.0001	0.0000	-0.0026
$3d_{5/2} \rightarrow 4d_{3/2}$	-0.0017	0.0001	-0.0099	-0.0002	0.0000	-0.0012
$3d_{5/2} \rightarrow 4d_{5/2}$	-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
$4d_{3/2} \rightarrow 4d_{5/2}$	-1.5491	0.0003	0.0000	0.0000	0.0153	-1.5485
$5d_{3/2} \rightarrow 5d_{5/2}$	-1.5492	0.0019	0.0001	0.0000	0.0147	-1.5479
$4s_{1/2} \rightarrow 5s_{1/2}$	0.0004	-0.0006	0.0560	0.0000	0.0004	-0.0687
$4p_{1/2} \rightarrow 4p_{3/2}$	-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	0.000	0.0002	-0.0248
$4p_{1/2} \rightarrow 5p_{3/2}$	-0.0059	0.0108	-0.0060	0.0000	-0.0000	0.0049