Ab initio calculations of 'forbidden' transition probabilities and lifetimes of low-lying states in V^{4+}

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(Dated: February 2, 2008)

Electric quadrupole (E2) and magnetic dipole (M1) transition amplitudes among the low-lying states of quadruply ionized vanadium V^{4+}, important in various field of experimental and astrophysics are presented very accurately. Most of these results are reported for the first time in the literature. Relativistic coupled-cluster theory with single, double and leading triple excitations has been employed for these calculations. Estimation of different correlation effects arising through the above formalism have been highlighted by studying core and valence electrons excitations to the excited states. The lifetime of the first excited D- state is found to be long.

I. INTRODUCTION

Electromagnetic 'forbidden' transitions, especially for lighter neutral systems and their iso-electronic companions, are of immense important in atomic experiments due to precise use of metastable states [1]. Some of these transitions correspond to relatively longer wavelengths compared to normal allowed transitions of same system provide information about the thermal Doppler effects in many physical systems [2]. Different astronomical features have only been possible to observe from infrared and radio transitions. Many of these forbidden transitions of quadruply ionized vanadium (V^{4+}) have been related to dominant features in the optical spectra of planetary nebulae and the aurora [3]. Similar transitions have been identified with the so called coronal lines emitted by the Sun [4]. Under certain circumstances, which prevail in astrophysics and low density laboratory tokamak plasmas, electric quadrupole (E2) and magnetic dipole (M1) transition lines gain intensity and can be used to infer information about plasma temperature and their dynamics [5]. The intensities of these transitions allow us to measure the concentration of impurity ions in

tokamak which originate in the high temperature interior of the discharge [5]. From many-body points of view, the importance of these results lies in the estimation of the accuracy of the electronic wave function through out the radial extent of the atomic systems by comparing the results with experimental measurements [6]. Also computed results are only means of estimations for many of these transitions wherever experimental measurements are difficult.

Here, we present calculated wavelengths and transition amplitudes of V^{4+} involving E2 and M1 radiative transition amplitudes which are important in astronomy (as mentioned above), plasma research and can be used in many experiments in atomic and solid state physics [8, 9, 13]. The study of forbidden transitions between the fine structure states of the low-lying D-states needs special attantion as they play important role in the doping of impurity in Al_2O_3 crystal which is used to study high-frequency acoustic phonon in crystal [10]. It is also a good candidate to study electron spin resonance [11] and electron paramagnetic resonance [12] in quartz material. The detail knowledge of the resonant core relaxation process of V^{+4} [14] need accurate results of energy levels of this ion and transition amplitudes among them.

One of the most correlation exhaustive many-body approaches, the relativistic coupled cluster method with singles, doubles and partially triples (RCCSD(T)) has been employed. This is non-perterbative in nature. We also intend to investigate the core-core and core-valence correlation contributions obtained from the RCCSD(T) method to the M1 and E2 transitions among the low-lying states.

For the one-valence (v) open shell system, the exact wave function can be expressed using the RCC approach as

$$|\Psi_v\rangle = e^T\{e^{S_v}\}|\Phi_v\rangle = e^T\{1+S_v\}|\Phi_v\rangle, \tag{1.1}$$

where the curly brackets represent the normal order form [15] and the reference state is defined by

$$|\Phi_v\rangle = a_v^\dagger|\Phi_{DF}\rangle \tag{1.2}$$

for the closed-shell Dirac-Fock (DF) state, $|\Phi_{DF}\rangle$, of V^{+5}.

In the above equation, the T and S_v operators are the RCC excitation operators associate with the closed and open shell hole-particle excitations, respectively [15, 16]. The computationally intensive parts in this approach is to consider non-linear terms which involve maximum four powers of single (T_1) and two powers of double (T_2) normal ordered core-excitation operators and products with valence-virtual single excitation operators. Computational features are found in the product of T_1 and T_2 with S_{1v} and S_{2v}, which represent single excitation operator from valence orbitals and

double excitations from core-valence orbitals, respectively [17]. Leading order triple excitations [17, 18] are obtained from the latter part. For computational simplicity, the T amplitudes are calculated first for the closed-shell V^{5+} then the corresponding valence orbitals are attached to calculate the V^{5+} wave functions for V^{4+} system [19].

The DF orbitals of V^{5+} are generated from the universal Gaussian type orbital (GTO) basis functions [31] using $\alpha_0 = 0.00825$ and $\beta = 2.91$. Number of DF orbitals for different symmetries used in the RCC calculations is based on convergent criteria of core correlation energy. There are 12, 10, 10, 9 and 8 active orbitals including all core electrons are considered in the RCCSD(T) calculations for $l = 0$, 1, 2, 3, 4 symmetries, respectively. Other higher energy orbitals are considered as inactive.

The matrix element of any operator D can be expressed using the RCC method as

$$\begin{aligned} D_{fi} &= \frac{\langle\Psi_f|D|\Psi_i\rangle}{\langle\Psi_f|\Psi_i\rangle} \\ &= \frac{\langle\Phi_f|\{1+S_f{}^\dagger\}e^{T^\dagger}De^T\{1+S_i\}|\Phi_i\rangle}{\langle\Phi_f|\{1+S_f{}^\dagger\}e^{T^\dagger}e^T\{1+S_i\}|\Phi_i\rangle}. \end{aligned} \tag{1.3}$$

The one-electron reduced matrix elements of M1 and E2 operators are given by [18, 20].

$$\langle j_f||q_m^{(M1)}||j_i\rangle = \langle j_f||C_m^{(1)}||j_i\rangle\frac{6}{\alpha k}\frac{\kappa_i+\kappa_f}{2}\left[\int dr j_1(kr)(P_{kf}Q_{ki}+Q_{kf}P_{ki})\right] \tag{1.4}$$

and

$$\langle j_f||q_m^{(E2)}||j_i\rangle = \langle j_f||C_m^{(2)}||j_i\rangle\frac{15}{k^2}\left[\int dr j_2(kr)(P_{kf}P_{ki}+Q_{kf}Q_{ki}) + j_3(kr)\frac{j_f-j_i-1}{3}(P_{kf}Q_{ki}+Q_{kf}P_{ki})\right] \tag{1.5}$$

respectively, where j_i stand for the total angular momentum and $\kappa_i == \pm\left(j_i+\frac{1}{2}\right)$ is relativistic angular momentum quantum numbers of the i^{th} electron orbital. The quantity $C_m^{(1)}$ is the Racah tensor [17] and $j_l(kr)$ is the spherical Bessel function of order l. P_{ki} and Q_{ki} are the large and small radial components of the Dirac wave functions.

The emission transition rate (in $sec^{(-1)}$) for the E1, E2 and M1 channels from state f to i are given by,

$$A_{f\to i}^{E1} = \frac{2.0261\times10^{18}}{\lambda^3[j_f]}S_{f\to i}^{E1} \tag{1.6}$$

$$A_{f\to i}^{E2} = \frac{1.11995\times10^{18}}{\lambda^5[j_f]}S_{f\to i}^{E2} \tag{1.7}$$

$$A_{f\to i}^{M1} = \frac{2.69735\times10^{13}}{\lambda^3[j_f]}S_{f\to i}^{M1}, \tag{1.8}$$

where $[j_f] = 2j_f + 1$ is the degeneracy of the f-state, S is the square of the transition amplitude of the transition operator D, and λ (in Å) are the corresponding transition wavelength.

The lifetime (in sec) of a particular state is the reciprocal of total transition probabilities arising from all possible electromagnetic spontaneous transitions to the lower energy levels [17]. In Paper-I, we have found excellent agreement between the experimental and computed ionization energies using the RCCSD(T) approach. The good agreement between length and velocity form electric dipole transition matrix elements in the above paper demonstrates the accuracy of our numerical approach. Lifetime of excited ststes have been obtained from these forbidden transition amplitudes reported here and allowed transition probabilities obtained from the same RCCSD(T) calculation as Paper-I. Table I, shows that the $3d_{5/2}$ state has long lifetime and it can be used as a potential metastable states required for many atomic experiments.

Ali and Kim [21] had calculated M1 and E2 transition probabilities between $3d$ and $4s$ states using Dirac-Fock single-configuration (DFSC) approximation. We have made comparison with them to our calculated results in Table II. The difference between the results are due to the inclusion of electron correlation effects through the RCCSD(T) method. It is clear from this table that the magnetic dipole matrix element between $3d_{3/2}$ and $4s$ was highly underestimated in the DFSC calculation.

TABLE I: Lifetime of the low-lying states in V^{4+}

States	Lifetimes (in sec.)
$3d_{5/2}$	3.84E+02
$4s_{1/2}$	4.55E-05
$4p_{1/2}$	1.99E-10
$4p_{3/2}$	1.97E-10
$4d_{3/2}$	3.77E-10
$4d_{5/2}$	3.01E-10
$4f_{5/2}$	1.20E-10
$4f_{7/2}$	6.97E-11

The effect of the unbound orbitals in the correlation calculation of the E2 and M1 transition probabilities in the framework of the RCC approach is studied quantitatively in Tables III and IV, respectively, which is reported first time in the literature to our knowledge. We have considered transitions involving excited states few close to and few comparatively away from the ground state. As expected, the effect is more on the higher excited states compared to the excited states those

TABLE II: Comparison of $3d \rightarrow 4s$ transition probabilities with DFSC calculations [21]

Transitions	A_{M1}(DFSC)	A_{M1} (RCC)	A_{E2} (DFSC)	A_{E2}(RCC)
$3d\ ^2D_{3/2} \rightarrow 4s\ ^2S_{1/2}$	4.21(-06)	2.19(-02)	8.56(+03)	4.42(+03)
$3d\ ^2D_{5/2} \rightarrow 4s\ ^2S_{1/2}$			1.27(+04)	6.60(+03)

are closed to the ground state. Point to note that effect is more in E2 transition amplitudes and that can be explained by the dependance of these transition amplitudes in the more diffused region compare to M1 transition amplitudes.

TABLE III: Effect of unbound orbitals of V^{4+} on electric quadrupole transition amplitude

Terms		Trans. Amplitudes	
		(with bound orb.)	(with all orb.)
$4s_{1/2}$	$\rightarrow 4d_{3/2}$	-5.8530	-5.7383
	$\rightarrow 4d_{5/2}$	7.1673	7.0272
$4d_{3/2}$	$\rightarrow 4d_{5/2}$	-6.1508	-5.9673
$6s_{1/2}$	$\rightarrow 4d_{3/2}$	0.7921	0.7101
	$\rightarrow 4d_{5/2}$	-0.9823	-0.8820
$4p_{1/2}$	$\rightarrow 4p_{3/2}$	-6.2963	-6.1510
	$\rightarrow 6p_{3/2}$	-0.1036	-0.2787
$4p_{3/2}$	$\rightarrow 6p_{3/2}$	-0.0327	-0.1949
	$\rightarrow 6p_{1/2}$	-0.0747	-0.2562
$6p_{1/2}$	$\rightarrow 6p_{3/2}$	-0.5787	-4.6953

Tables V and VI give the magnetic dipole and electric quadrupole transition amplitudes, respectively, for most of the low-lying states. They are all relevant astrophysically. The important transitions among these from the physics point of view are forbidden transitions among fine-structure states of $3d$ and $4p$. Former one falls in the infrared region, which has many applications in plasma research and infrared laser spectroscopy [22] and latter one falls in the optical region, has immense prospect in different atomic physics experiments. We have not reported wavelength comparison for most of other fine structure transitions fall far beyond the infrared region. The relatively large differences in the wavelengths between some of the transitions from $4f$ states call for further experimental and theoretical investigations on these states.

Quantitative contributions from different correlation terms for few M1 and E2 transitions among

TABLE IV: Effect of unbound orbitals of V^{4+} on magnetic dipole transition amplitude

Terms		Transition Amplitude	
		(with bound orb.)	(with all orb.)
$4s_{1/2}$	$\rightarrow 6s_{1/2}$	-0.0126	-0.0227
$4d_{3/2}$	$\rightarrow 4d_{5/2}$	-1.5485	-1.5455
$4p_{1/2}$	$\rightarrow 4p_{3/2}$	-1.1544	-1.1535
	$\rightarrow 6p_{1/2}$	-0.0102	-0.0116
	$\rightarrow 6p_{3/2}$	0.0071	0.0072
$4p_{3/2}$	$\rightarrow 6p_{1/2}$	-0.0082	-0.0055
	$\rightarrow 6p_{3/2}$	-0.0746	-0.0820
$6p_{1/2}$	$\rightarrow 6p_{3/2}$	-1.5398	-1.5398

low laying states are presented in tables VII, VIII and IX. These tables shows comparative estimations of core polarisation, core correlation and pair correlation for these transitions. These tables show that core-polarization effects ($\overline{D}S_{2i}$) coming from the initial state for all the transitions are negligible. Wheras the combined effects of S_2 operators of both initial and final states contributing significant for both M1 and E2 transitions amplitudes.

II. CONCLUSION

Lifetimes of the low-lying bound states of V^{+4} have been calculated using highly correlated relativistic coupled-cluster approach. Long lifetimes have been observed for the first excited D-states and they can be used as potential metastable state for experiments in physics. Magnetic dipole and electric quadrupole transition amplitudes among bound states of the system, important for astronomical observations and plasma researches are estimated for the first time in the literature for most of the cases. 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. We have also highlighted different correlation effects arising through the RCCSD(T) method.

III. ACKNOWLEDGMENT

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TABLE V: Transition wavelengths and transition amplitudes of V^{4+} for magnetic dipole transitions.

Transitions		λ_{NIST}(Å)	λ_{RCC}(Å)	Transition amplitudes
$3d_{3/2}$	$\rightarrow 3d_{5/2}$			-1.5398
	$\rightarrow 4d_{3/2}$	340.24	340.22	0.0684
	$\rightarrow 4d_{5/2}$	340.08	340.04	0.0022
	$\rightarrow 5d_{3/2}$	257.74	257.58	-0.0362
	$\rightarrow 5d_{5/2}$	257.70	257.53	-0.0006
	$\rightarrow 6d_{3/2}$	230.25	230.08	-0.0219
	$\rightarrow 6d_{5/2}$	230.23	230.06	-0.0001
	$\rightarrow 4s_{1/2}$	675.02	684.25	0.0010
	$\rightarrow 5s_{1/2}$	304.67	306.30	-0.0004
	$\rightarrow 6s_{1/2}$	247.61	248.25	-0.0002
$3d_{5/2}$	$\rightarrow 4d_{3/2}$	340.97	341.04	-0.0062
	$\rightarrow 4d_{5/2}$	340.80	340.86	0.1860
	$\rightarrow 5d_{3/2}$	258.16	258.05	0.0027
	$\rightarrow 5d_{5/2}$	258.11	258.00	-0.0984
	$\rightarrow 6d_{3/2}$	230.58	230.45	0.0013
	$\rightarrow 6d_{5/2}$	230.56	230.44	-0.0598
$4d_{3/2}$	$\rightarrow 4d_{5/2}$			-1.5455
	$\rightarrow 5d_{3/2}$	1062.99	1063.24	-0.1248
	$\rightarrow 5d_{5/2}$	1062.23	1062.49	-0.0015
	$\rightarrow 6d_{3/2}$	712.24	712.36	-0.0540
	$\rightarrow 6d_{5/2}$	712.05	712.17	0.0008
$4d_{5/2}$	$\rightarrow 5d_{3/2}$	1064.62	1062.18	0.0050
	$\rightarrow 5d_{5/2}$	1063.86	1061.36	-0.3485
	$\rightarrow 6d_{3/2}$	712.97	711.53	0.0006
	$\rightarrow 6d_{5/2}$	712.79	711.38	-0.1508
$5d_{3/2}$	$\rightarrow 5d_{5/2}$			-1.5436
	$\rightarrow 6d_{3/2}$	2158.58	2155.39	0.1210
	$\rightarrow 6d_{5/2}$	2142.40	2153.97	0.0012
$5d_{5/2}$	$\rightarrow 6d_{3/2}$	2161.69	2158.76	-0.0044
	$\rightarrow 6d_{5/2}$	2159.95	2157.34	-0.0044
$6d_{3/2}$	$\rightarrow 6d_{5/2}$			-1.5453
$4s_{1/2}$	$\rightarrow 5s_{1/2}$	555.32	554.40	-0.5404
	$\rightarrow 6s_{1/2}$	391.06	389.52	-0.0227
$5s_{1/2}$	$\rightarrow 6s_{1/2}$	1322.08	1309.81	0.0496
$4p_{1/2}$	$\rightarrow 4p_{3/2}$	78971.47	77464.73	-1.1535
	$\rightarrow 5p_{1/2}$	689.14	688.02	-0.0207
	$\rightarrow 5p_{3/2}$	689.69	685.73	0.0053
	$\rightarrow 6p_{1/2}$	478.40	478.18	-0.0116

Transitions		λ_{NIST}(Å)	λ_{RCC}(Å)	Transition amplitudes
$4p_{3/2}$	$\rightarrow 5p_{1/2}$	695.21	694.18	0.0072
	$\rightarrow 5p_{3/2}$	692.72	691.85	-0.1305
	$\rightarrow 6p_{1/2}$	481.32	481.15	-0.0055
	$\rightarrow 6p_{3/2}$	480.73	481.20	-0.0820
$5p_{1/2}$	$\rightarrow 5p_{3/2}$			-1.1530
	$\rightarrow 6p_{1/2}$	1564.46	1567.89	0.0179
	$\rightarrow 6p_{3/2}$	1558.23	1568.41	-0.0077
$5p_{3/2}$	$\rightarrow 6p_{1/2}$	1577.24	1579.91	0.0061
	$\rightarrow 6p_{3/2}$	1570.91	1580.45	0.1222
$6p_{1/2}$	$\rightarrow 6p_{3/2}$			-1.4409
$4f_{5/2}$	$\rightarrow 4f_{7/2}$			1.8435
$5g_{7/2}$	$\rightarrow 5g_{9/2}$			-2.1081
	$\rightarrow 6g_{7/2}$	2970.51	2850.75	0.0379
	$\rightarrow 6g_{9/2}$	2970.45	2851.10	-0.0001
$5g_{9/2}$	$\rightarrow 6g_{7/2}$	2970.64	2850.29	0.0000
	$\rightarrow 6g_{9/2}$	2970.58	2850.64	0.0663
$6g_{7/2}$	$\rightarrow 6g_{9/2}$			-2.1080

TABLE VI: Transition wavelengths and transition amplitudes of V^{4+} for electric quadrupole transitions.

Transitions		λ_{NIST}(Å)	$\lambda_{RCCSD(T)}$(Å)	Transition amplitudes
$3d_{3/2}$	$\rightarrow 3d_{5/2}$			-0.7475
	$\rightarrow 4d_{3/2}$	340.24	340.22	1.0870
	$\rightarrow 4d_{5/2}$	340.08	341.71	0.7290
	$\rightarrow 5d_{3/2}$	257.74	258.63	-0.3948
	$\rightarrow 5d_{5/2}$	257.70	258.53	-0.2659
	$\rightarrow 6d_{3/2}$	230.25	230.95	-0.1950
	$\rightarrow 6d_{5/2}$	230.23	230.93	-0.1321
	$\rightarrow 4s_{1/2}$	675.02	684.25	-1.4876
	$\rightarrow 5s_{1/2}$	304.67	306.30	0.0683
	$\rightarrow 6s_{1/2}$	247.61	248.25	0.0269
	$\rightarrow 5g_{7/2}$	240.17	240.98	-0.8463
	$\rightarrow 6g_{7/2}$	222.21	222.19	-0.6366
$3d_{5/2}$	$\rightarrow 4d_{3/2}$	340.97	341.04	-0.7357
	$\rightarrow 4d_{5/2}$	340.80	340.86	1.4290
	$\rightarrow 5d_{3/2}$	258.16	258.05	0.2682
	$\rightarrow 5d_{5/2}$	258.11	258.00	-0.5192
	$\rightarrow 6d_{3/2}$	230.58	230.45	0.1337
	$\rightarrow 6d_{5/2}$	230.56	230.44	-0.2574
	$\rightarrow 4s_{1/2}$	677.88	680.17	-1.8310
	$\rightarrow 5s_{1/2}$	305.25	305.44	0.0829
	$\rightarrow 6s_{1/2}$	247.99	247.68	0.0329
	$\rightarrow 5g_{7/2}$	240.53	241.39	0.2839
	$\rightarrow 5g_{9/2}$	240.53	241.39	-1.0037
	$\rightarrow 6g_{7/2}$	222.51	222.54	0.2133
	$\rightarrow 6g_{9/2}$	222.51	222.55	-0.7539
$4d_{3/2}$	$\rightarrow 4d_{5/2}$			-5.9673
	$\rightarrow 5d_{3/2}$	1062.99	1060.41	-5.5444
	$\rightarrow 5d_{5/2}$	1062.23	1059.60	-3.8912
	$\rightarrow 6d_{3/2}$	712.24	710.74	-1.8378
	$\rightarrow 6d_{5/2}$	712.05	710.59	-1.3032
	$\rightarrow 4s_{1/2}$	686.06	684.00	5.7383
	$\rightarrow 5s_{1/2}$	2914.22	2925.88	9.4581
	$\rightarrow 6s_{1/2}$	909.48	904.77	-0.7101
	$\rightarrow 5g_{7/2}$	816.61	826.14	16.3355
	$\rightarrow 6g_{7/2}$	640.52	640.52	6.1353

Transitions		λ_{NIST}(Å)	$\lambda_{RCCSD(T)}$(Å)	Transition amplitudes
$4d_{5/2}$	$\rightarrow 5d_{3/2}$	1064.62	1062.18	3.9140
	$\rightarrow 5d_{5/2}$	1063.86	1061.36	-7.2728
	$\rightarrow 6d_{3/2}$	712.97	711.53	1.3062
	$\rightarrow 6d_{5/2}$	712.79	711.38	-2.4142
	$\rightarrow 4s_{1/2}$	685.38	683.27	7.0272
	$\rightarrow 5s_{1/2}$	2926.53	2939.35	11.6086
	$\rightarrow 6s_{1/2}$	910.68	906.06	-0.8820
	$\rightarrow 5g_{7/2}$	817.57	827.21	-5.4566
	$\rightarrow 5g_{9/2}$	817.56	827.25	19.2923
	$\rightarrow 6g_{7/2}$	641.11	641.16	-2.0469
	$\rightarrow 6g_{9/2}$	641.12	641.18	7.2372
$5d_{3/2}$	$\rightarrow 5d_{5/2}$			-19.0483
	$\rightarrow 6d_{3/2}$	2158.58	2155.39	15.9663
	$\rightarrow 6d_{5/2}$	2156.85	2153.97	11.2383
	$\rightarrow 4s_{1/2}$	416.95	415.80	0.1076
	$\rightarrow 5s_{1/2}$	1673.36	1663.21	18.2095
	$\rightarrow 6s_{1/2}$	6298.00	6164.49	-29.2917
	$\rightarrow 5g_{7/2}$	3523.20	3739.47	44.8003
	$\rightarrow 6g_{7/2}$	1611.66	1617.59	-27.9356
$5d_{5/2}$	$\rightarrow 6d_{3/2}$	2161.69	2158.76	-11.3019
	$\rightarrow 6d_{5/2}$	2159.95	2157.34	20.9536
	$\rightarrow 4s_{1/2}$	416.83	415.67	0.1240
	$\rightarrow 5s_{1/2}$	1671.50	1661.21	22.2903
	$\rightarrow 6s_{1/2}$	6324.53	6192.12	-35.9371
	$\rightarrow 5g_{7/2}$	3531.49	3749.62	-14.9385
	$\rightarrow 5g_{9/2}$	3531.31	3770.43	52.8170
	$\rightarrow 6g_{7/2}$	1613.40	1619.49	9.3478
	$\rightarrow 6g_{9/2}$	1613.38	1619.60	-33.0483
$6d_{3/2}$	$\rightarrow 6d_{5/2}$			-49.7139
	$\rightarrow 4s_{1/2}$	349.45	348.55	0.1295
	$\rightarrow 5s_{1/2}$	942.62	938.79	0.5210
	$\rightarrow 6s_{1/2}$	3284.21	3314.19	47.8467
	$\rightarrow 5g_{7/2}$	5573.05	5088.16	-29.2475
	$\rightarrow 6g_{7/2}$	6361.01	6483.01	128.4251
$6d_{5/2}$	$\rightarrow 4s_{1/2}$	349.40	348.52	0.1553
	$\rightarrow 5s_{1/2}$	942.29	938.52	0.6557
	$\rightarrow 6s_{1/2}$	3280.21	3310.84	58.5607
	$\rightarrow 5g_{7/2}$	5561.54	5080.26	9.7363
	$\rightarrow 5g_{9/2}$	5562.00	5078.78	-34.4251

Transitions		λ_{NIST}(Å)	$\lambda_{RCCSD(T)}$(Å)	Transition amplitudes
$5g_{7/2}$	$\rightarrow 5g_{9/2}$			-14.0132
	$\rightarrow 6g_{7/2}$	2970.51	2850.75	25.5408
	$\rightarrow 6g_{9/2}$	2970.45	2851.10	7.7503
$5g_{9/2}$	$\rightarrow 6g_{7/2}$	2970.64	2850.29	-7.7543
	$\rightarrow 6g_{9/2}$	2970.58	2850.64	28.8149
$6g_{7/2}$	$\rightarrow 6g_{9/2}$			-44.2007
$4p_{1/2}$	$\rightarrow 4p_{3/2}$	78971.47	77464.73	-6.1510
	$\rightarrow 5p_{3/2}$	686.69	685.73	-3.5604
	$\rightarrow 6p_{3/2}$	477.82	478.23	-0.2787
	$\rightarrow 4f_{5/2}$	697.92	709.04	8.4251
$5p_{1/2}$	$\rightarrow 4p_{3/2}$	695.21	694.18	-3.6670
	$\rightarrow 5p_{3/2}$			-21.5598
	$\rightarrow 6p_{3/2}$	1558.23	1568.41	2.9529
	$\rightarrow 4f_{5/2}$	54796.32	23207.88	13.7048
$6p_{1/2}$	$\rightarrow 4p_{3/2}$	481.32	481.15	-0.2562
	$\rightarrow 5p_{3/2}$	1577.24	1579.91	3.0066
	$\rightarrow 6p_{3/2}$			-4.6953
	$\rightarrow 4f_{7/2}$	1521.03	1468.67	-0.7073
$4p_{3/2}$	$\rightarrow 5p_{3/2}$	692.72	691.85	-3.4660
	$\rightarrow 6p_{3/2}$	480.73	481.20	-0.1949
	$\rightarrow 4f_{5/2}$	704.14	715.59	-4.5351
	$\rightarrow 4f_{7/2}$	706.25	715.71	-11.0889
$5p_{3/2}$	$\rightarrow 6p_{3/2}$	1570.91	1580.45	2.6031
	$\rightarrow 4f_{5/2}$	37839.08	20858.40	-7.3110
	$\rightarrow 4f_{7/2}$	32616.42	20755.93	-17.8582
$6p_{3/2}$	$\rightarrow 4f_{5/2}$	1515.14	1469.13	0.3491
	$\rightarrow 4f_{7/2}$	1505.49	1468.62	0.8998
$4f_{5/2}$	$\rightarrow 4f_{7/2}$			5.5868

RCC terms	$3d_{3/2} \rightarrow 3d_{5/2}$	$3d_{3/2} \rightarrow 4d_{3/2}$	$3d_{3/2} \rightarrow 4s_{1/2}$	$3d_{3/2} \rightarrow 5s_{1/2}$	$3d_{3/2} \rightarrow 5g_{7/2}$	$3d_{5/2} \rightarrow 4d_{3/2}$	$3d_{5/2} \rightarrow 4s_{1/2}$	$3d_{5/2} \rightarrow 5s_{1/2}$	$3d_{5/2} \rightarrow 5g_{7/2}$
Dirac-Fock D	-0.8554	1.1077	-1.5552	0.0624	-0.9137	-0.7289	-1.9121	0.0748	0.3061
$\overline{D}$	-0.8466	1.1079	-1.5505	0.0604	-0.9125	-0.7287	-1.9060	0.0722	0.3057
$\overline{D}S_{1i}$	0.0180	-0.0896	0.0882	0.0284	0.0774	0.0585	0.1078	0.0348	-0.0257
$S_{1f}^{\dagger}D$	0.0178	0.0252	-0.0019	-0.0351	-0.0096	-0.0355	-0.0023	-0.0432	0.0032
$\overline{D}S_{2i}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{2f}^{\dagger}D$	0.0625	0.0501	-0.0244	0.0092	-0.0036	-0.0337	-0.0318	0.0124	0.0014
$S_{1f}^{\dagger}\overline{D}S_{1i}$	0.0000	-0.0012	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{1f}^{\dagger}\overline{D}S_{2i}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{2f}^{\dagger}\overline{D}S_{1i}$	0.0001	0.0010	-0.0013	0.0006	-0.0004	-0.0006	-0.0016	0.0007	0.0001
$S_{2f}^{\dagger}\overline{D}S_{2i}$	-0.0078	0.0039	-0.0104	0.0048	-0.0021	-0.0026	-0.0127	0.0053	0.0006
Important effective two-body terms of $\overline{D}$									
$S_{2f}^{\dagger}DT_1$	0.0003	0.0002	0.0002	-0.0001	0.0000	-0.0002	0.0002	-0.0001	0.0000
$T_1^{\dagger}DS_{2i}$	0.0003	0.0000	0.0001	0.0000	0.0000	0.0000	0.0002	-0.0001	0.0000
$T_2^{\dagger}DS_{2i}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{2f}^{\dagger}DT_2$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0026	0.0015	0.0000
Norm.	0.0075	-0.0107	0.0143	-0.0004	0.0044	0.0072	0.0175	-0.0005	-0.0014

TABLE VII: Explicit contributions from the RCCSD(T) calculations to the absolute magnitude of reduced E2 transitions matrix elements in a.u.

RCC terms	$3d_{5/2} \rightarrow 5g_{9/2}$	$4d_{3/2} \rightarrow 4s_{1/2}$	$4d_{3/2} \rightarrow 5s_{1/2}$	$4d_{3/2} \rightarrow 5g_{7/2}$	$4p_{1/2} \rightarrow 4p_{3/2}$	$4p_{1/2} \rightarrow 4f_{5/2}$	$4p_{3/2} \rightarrow 4f_{5/2}$	$4p_{3/2} \rightarrow 4f_{7/2}$	$4f_{5/2} \rightarrow 5f_{7/2}$
Dirac-Fock D	-1.0825	5.9612	10.0120	17.4676	-6.4365	9.1096	-4.9059	-12.0170	6.5586
$\overline{D}$	-1.0810	5.9612	10.0120	17.4678	-6.4367	9.1094	-4.9061	-12.0174	6.5585
$\overline{D}S_{1i}$	0.0912	0.0177	-0.6124	-1.0685	0.1011	-0.2782	0.1485	0.3639	-0.2998
$S_{1f}^{\dagger}D$	-0.0110	-0.1701	0.1189	0.0334	0.0982	-0.0815	0.0463	0.1145	-0.3017
$\overline{D}S_{2i}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{2f}^{\dagger}D$	-0.0047	-0.0430	0.0060	-0.0264	0.0654	-0.0557	0.0302	0.0733	-0.0195
$S_{1f}^{\dagger}\overline{D}S_{1i}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{1f}^{\dagger}\overline{D}S_{2i}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{2f}^{\dagger}\overline{D}S_{1i}$	-0.0005	-0.0010	0.0010	0.0001	0.0007	-0.0002	0.0001	0.0003	-0.0011
$S_{2f}^{\dagger}\overline{D}S_{2i}$	-0.0026	0.0277	-0.0013	0.0113	-0.0316	0.0479	-0.0245	-0.0614	0.0389
Important effective two-body terms of $\overline{D}$									
$S_{2f}^{\dagger}DT_1$	0.0000	-0.0002	0.0001	0.0000	0.0003	-0.0001	0.0000	0.0001	0.0000
$T_1^{\dagger}DS_{2i}$	0.0000	-0.0001	0.0001	0.0000	0.0000	-0.0003	0.0001	0.0003	0.0000
$T_2^{\dagger}DS_{2i}$	0.0000	0.0000	0.0000	0.0000	0.0055	0.0029	-0.0017	-0.0040	0.0000
$S_{2f}^{\dagger}DT_2$	0.0000	0.0003	-0.0002	0.0000	-0.0025	0.0000	0.0000	0.0000	0.0000
Norm.	0.0051	-0.0543	-0.0657	-0.0822	0.0557	-0.3186	0.1714	0.4418	-0.3881

TABLE VIII: Explicit contributions from the RCCSD(T) calculations to the absolute magnitude of reduced E2 transitions matrix elements in a.u.

RCC terms	$3d_{3/2} \rightarrow 3d_{5/2}$	$3d_{3/2} \rightarrow 4d_{3/2}$	$4s_{1/2} \rightarrow 5s_{1/2}$	$4p_{1/2} \rightarrow 4p_{3/2}$	$4f_{5/2} \rightarrow 4f_{7/2}$	$5g_{7/2} \rightarrow 5g_{9/2}$
Dirac-Fock D	-1.5489	-0.0004	0.0004	-1.1545	1.8515	-2.1081
$\overline{D}$	-1.5291	-0.0020	0.0015	-1.1538	1.8515	-2.1081
$\overline{D}S_{1i}$	0.0001	0.0511	-0.0440	0.0002	0.0000	0.0000
$S_{1f}^{\dagger}D$	0.0000	0.0000	0.0000	-0.0002	0.0000	0.0000
$\overline{D}S_{2i}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{2f}^{\dagger}\overline{D}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{1f}^{\dagger}\overline{D}S_{1i}$	0.0000	0.0017	-0.0006	0.0000	0.0000	0.0000
$S_{1f}^{\dagger}\overline{D}S_{2i}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{2f}^{\dagger}\overline{D}S_{1i}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{2f}^{\dagger}\overline{D}S_{2i}$	-0.0187	0.0199	-0.0118	-0.0106	0.1203	-0.0008
Important effective two-body terms of $\overline{D}$						
$S_{2f}^{\dagger}DT_1$	0.0011	-0.0009	0.0002	0.0001	0.0000	0.0000
$T_1^{\dagger}DS_{2i}$	0.0011	-0.0006	0.0001	0.0001	0.0000	0.0000
$T_2^{\dagger}DS_{2i}$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$S_{2f}^{\dagger}DT_2$	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Norm.	0.0154	-0.0006	0.0003	0.0104	-0.1280	0.0008

TABLE IX: Explicit contributions from the RCCSD(T) calculations to the absolute magnitude of reduced M1 transitions matrix elements in a.u.