Ab initio calculations of oscillator strengths and lifetimes of low-lying states in Mo VI

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(Dated: August 2, 2010)

Relativistic coupled-cluster (RCC) calculations have been performed to estimate the electromagnetic forbidden transition probabilities, oscillator strengths and lifetimes of many low-lying states of five times ionized molybdenum (Mo VI). Contributions from the Breit interaction up to the first order of perturbation have been examined. Our results are in good agreement with the available other reported theoretical and experimental results. A long lifetime about 4.9854 s of the first excited state, 4d²D₅/₂, has been predicted which can be a very useful criteria in the doping process of thin films. Correlations trends from various RCC terms to the transition amplitude calculations are discussed.

I. INTRODUCTION

Electromagnetic forbidden, both magnetic dipole (M1) and electric quadrupole (E2), transitions of Mo VI are important for temperature and density estimations of tokamak plasmas [1, 2], especially in the collision-radiative model [3, 4]. Long lifetimes of metastable states are dominated by these forbidden transitions and these states are generally difficult to observe in the laboratory plasmas due to strong collisions. However, these forbidden transitions of Mo VI have been observed in laboratory in electron spin resonance experiment [5] and therefore, they must be one of the sources of density estimations in astrophysical plasmas where collisions are very low due to high dilute interstellar medium [6]. Accurate estimation of abundances of molybdenum in the atmosphere of the evolved stars are important to understand the stellar nucleosynthesis [7].

Hexavelent molybdenum, isoelectronic to rubidium with 4p⁶4d as ground state configu-
ration, is generated by electron impact in the atomic collision process. The electron-impact ionization of multiply charged Mo ions, relevant to astrophysics and laboratory plasma research, have also been investigated [8]. Recently, Fisker et al. have given the possibility of the origin of the lightest isotope of molybdenum in proton rich type II supernova [9]. The necessity of accurate estimation of allowed dipole transition strengths to find out their mixing these effects in the dipole forbidden transitions in Mo VI is explicitly discussed by T. Yamamoto [10]. Again, the transition strength between the fine structure states of 4d level can reflect the electronic structure of Mo VI in crystal [11].

A few calculations have been carried out to study the on electric dipole (E1) transitions in Mo VI over the last few decades using the mean-field theory [12, 13]. More recently, J. Reader [15] has estimated the E1 transition probabilities among low-lying states by estimating transition strengths in the semiempirical approach with the experimental excitation energies.

For this single reference system, Mo VI, we have performed relativistic coupled-cluster (RCC) calculation with single (S), double (D) and partial triple (T) excitations in the framework of Fock space multi-reference (FSMR). Both the excitation energies and transition probabilities are determined using this RCC method using which lifetimes of many low-lying states are estimated.

II. THEORY AND METHOD OF CALCULATIONS

A. Theory

The oscillator strength for E1 transition from \(|\Psi_f\rangle\) to \(|\Psi_i\rangle\) is given as

\[
f_{fi} = \frac{2}{3g_f} \Delta E_{fi} \times |D_{fi}|^2,
\]

(2.1)

where \(\Delta E_{fi}\) is the excitation energy between the upper and lower states and \(g_f = 2J_f + 1\) is the degeneracy factor of the upper state with total angular momentum \(J_f\).

The single particle reduced matrix elements for the E1, E2 and M1 transition operators are given in [21]. The emission transition probabilities (in sec\(^{-1}\)) for the E1, E2 and M1 channels from states \(f\) to \(i\) can be expressed as

\[
A_{fi}^{E1} = \frac{2.0261 \times 10^{18}}{\lambda^3(2j_f + 1)} S_{E1},
\]

(2.2)
\[ A_{fi}^{E2} = \frac{1.11995 \times 10^{18}}{\lambda^5(2j_f + 1)} S_{E2}, \quad (2.3) \]

\[ A_{fi}^{M1} = \frac{2.69735 \times 10^{13}}{\lambda^3(2j_f + 1)} S_{M1}, \quad (2.4) \]

where \( S^O = |\langle \Psi_f | O | \Psi_i \rangle|^2 \) is the transition strength for the corresponding operator \( O \) (in a.u.) and \( \lambda \) (in Å) is the corresponding transition wavelength.

The lifetime of a particular excited state \( i \) can be computed by the reciprocal of the total transition probability, \( \sum_j A_{ij} \) (in sec\(^{-1}\)), arising from all possible states \( j \) due to spontaneous electromagnetic transitions, i.e.

\[ \tau_i = \frac{1}{\sum_j A_{ij}}. \quad (2.5) \]

**B. Fock Space Multi-reference RCC theory**

The FSMRCC method is one of the most powerful highly correlated many-body approaches due to its all order structure to account the correlation effects [16]. The FSMRCC, which is mainly meant for multi-reference systems, is used here for the one valence electron and has been described in details elsewhere [16–19]. Here we present the method briefly.

We first consider the Dirac-Coulomb Hamiltonian for a closed-shell \( N \) electron system which is given by

\[ H = \sum_{i=1}^{N} \left[ \alpha \vec{\alpha}_i \cdot \vec{p}_i + \beta mc^2 + V_{\text{Nuc}}(r_i) \right] + \sum_{i<j} \frac{1}{r_{ij}}, \quad (2.6) \]

with all the standard notations often used.

The theory for a single valence system is based on the concept of common vacuum for both the closed shell \( N \)- and open shell \( N \pm 1 \)-electron systems, which allows us to formulate a direct method to determine energy differences (electron attachment energy or negative of the ionization potential). Also, the holes and particles are defined with respect to the common vacuum for both the electron systems. Model space of an \((n,m)\) Fock-space contains determinants of \( n \) holes and \( m \) particles distributed within a set of orbitals known as *active* orbitals. For example, in the present article, we are dealing with \((0,1)\) Fock-space which is a complete model space (CMS) by construction and is given by

\[ |\Psi^{(0,1)}\rangle = \sum_i C_{ij\mu} |\Phi_i^{(0,1)}\rangle, \quad (2.7) \]
where \( C_{\mu} \)'s are the expansion coefficients of \( \Psi_{\mu}^{(0,1)} \), and \( \Phi_{i}^{(0,1)} \)'s are the model space configurations made of DF orbitals. The dynamical electron correlation effects are introduced through the *valence-universal* wave-operator \( \Omega \) \[16, 17\]

\[
\Omega = \{ \exp(\tilde{S}) \}, \tag{2.8}
\]

where

\[
\tilde{S} = \sum_{k=0}^{m} \sum_{l=0}^{n} S^{(k,l)} = S^{(0,0)} + S^{(0,1)} + S^{(1,0)} + \ldots \tag{2.9}
\]

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 \( \Omega \) is in normal ordered, we can rewrite Eq. \( 2.8 \) as

\[
\Omega = \exp(T)\{ \exp(S) \}. \tag{2.10}
\]

The “valence-universal” wave-operator \( \Omega \) in Eq. \( 2.10 \) is parameterized in such a way that the states generated by its action on the reference space satisfy the Fock-space Bloch equation

\[
H\Omega P(k,l) = \Omega P(k,l)H_{\text{eff}}P(k,l), \tag{2.11}
\]

where

\[
H_{\text{eff}} = P(k,l)H\Omega P(k,l). \tag{2.12}
\]

Here, \( P \) is the projection operator of model space. Eq. \( 2.11 \) is valid for all \( (k,l) \) starting from \( k=l=0 \) (i.e., the core problem) to some desired parent model space, with \( k=m, l=n \). In this present calculation, we truncate Eq. \( 2.9 \) at \( m=0 \) and \( n=1 \).

In this work, single \( (T_1, S_{1}^{(0,1)}) \) and double \( (T_2, S_{2}^{(0,1)}) \) excitations are considered for \( T \) and \( S \) clusters operator. Therefore, the total correlated wavefunction of the system with single valence orbital \( v \), can be written as

\[
|\Psi_{v}\rangle = \Omega|\Psi^{(0,0)}\rangle = e^{T_1+T_2}\{1 + S_{1v}^{(0,1)} + S_{2v}^{(0,1)}\}|\Psi^{(0,0)}\rangle. \tag{2.13}
\]

Important triple excitations, correspond to the correlation to the valence orbitals, are included in the open shell FSMRCC-SD calculations by an approximation that is similar in spirit to FSMRCC-SD(T) \[20\]. The approximate valence triple excitation amplitudes are given by

\[
S_{v(0,1)abk}^{pqr} = \frac{\langle \widehat{V_{2}} \rangle_{pab}^{qrr} + \langle \widehat{V_{1}} S_{2v}^{(0,1)} \rangle_{pab}^{qrr}}{\varepsilon_{a} + \varepsilon_{b} + \varepsilon_{k} - \varepsilon_{p} - \varepsilon_{q} - \varepsilon_{r}}, \tag{2.14}
\]
where $S_{v(0,1)abk}$ are the amplitudes corresponding to the simultaneous excitations from core orbitals $a, b$ and valence $k$ to virtual orbitals $p, q$, and $r$, respectively. $VT_2$ and $VS_{2v}^{(0,1)}$ are the connected composites involving $V$ and $T$, and $V$ and $S_{v}^{(0,1)}$, respectively, where $V$ is the two electron Coulomb ($\frac{1}{r_{ij}}$) integral and $\varepsilon$’s are the orbital energies.

The transition matrix element due to any operator $O$ can be expressed as

$$O_{fi} = \frac{\langle \Phi_{f} | \{ 1 + S_{f}^{(0,1)} \} e^{T^\dagger} O e^{T} \{ 1 + S_{i}^{(0,1)} \} | \Phi_{i} \rangle \sqrt{\langle \Phi_{f} | \{ 1 + S_{f}^{(0,1)} \} e^{T^\dagger} e^{T} \{ 1 + S_{f}^{(0,1)} \} | \Phi_{f} \rangle}}{\langle \Psi_{f} | O | \Psi_{f} \rangle \langle \Psi_{i} | \Psi_{i} \rangle}$$

$$= \frac{\langle \Phi_{f} | \{ 1 + S_{f}^{(0,1)} \} e^{T^\dagger} e^{T} \{ 1 + S_{i}^{(0,1)} \} | \Phi_{i} \rangle \langle \Phi_{i} | \{ 1 + S_{i}^{(0,1)} \} e^{T^\dagger} e^{T} \{ 1 + S_{i}^{(0,1)} \} | \Phi_{i} \rangle}{\langle \Psi_{f} | \{ 1 + S_{f}^{(0,1)} \} e^{T^\dagger} e^{T} \{ 1 + S_{i}^{(0,1)} \} | \Psi_{f} \rangle}.$$  

(2.15)

### III. RESULTS AND DISCUSSIONS

In the present calculation, the radial wavefunctions of DF orbitals of closed shell Mo VII are obtained using Gaussian type orbitals (GTO) basis with finite nuclear size as discussed in our earlier paper \[22\]. We have used universal basis set, where the exponent $\alpha_i$ is related with two parameters $\alpha_0$ and $\beta$, same for all the symmetries, expressed as

$$\alpha_i = \alpha_0 \beta^{i-1}. \quad (3.1)$$

We have considered $\alpha_0$ and $\beta$ as 0.00625 and 2.72, respectively, after obtaining best fit of the bound orbital energies and evaluating the expectation values of different radial functions ($r$, $r^2$, $1/r$) generated with GTOs and GRASP2 \[23\]. In the DF calculations, we have taken 22, 20, 17, 15, and 12 number of GTOs for s, p, d, f, and g type symmetries, respectively, to generate the atomic orbitals. In Fig. 1 we have given the relative errors obtained for different orbitals in the calculations of these quantities using the above chosen parameters. Since these errors are very small, it shows that there is a good agreement between results. We assume that both the bound and continuum orbitals generated using the above parameters will describe well both inside and outside of the nucleus. Therefore, we have considered all the orbitals obtained using GTOs for the rest of the calculations.

The number of the DF orbitals for different symmetries used in the present calculation is based on convergent criteria of core correlation energy of Mo VII for which it satisfies numerical completeness. The number of DF orbitals considered for s, p, d, f, and g type
symmetries in the RCC calculations are 12, 11, 10, 9 and 8, respectively; and among them 9, 8, 7, 5, and 5 are bound orbitals, respectively, including all the core orbitals. The $T$ amplitudes are first determined by solving the closed shell RCC equations for the closed-shell system (Mo VII), then $S$ amplitudes are solved from the open-shell equations for the single-valence states of Mo VI.

Table I summarizes the calculated excitation energies (EE) and fine structure splitting (FS) of low-lying excited states and their comparison with the recent experimental results [15]. The average deviation is around 0.5% for EE. We have also presented the contribution from the partial triple excitations to the EE ($E_{\text{triple}}$), which is around 0.3% to the total EE. We have examined the first order excitation energy corrections due to Breit interaction using large scale relativistic CI calculations. Maximum contribution is coming for 5s state, which is around $+2\%$, whereas, contributions to 5p and 4f states are around $+0.4\%$ and $-0.04\%$; respectively. For 5d state, it is as small as 54 $cm^{-1}$ consistent with the result obtained by

FIG. 1: The relative energies and expectation values of $r$, $r^2$ and $1/r$ of the DF GTO orbitals to the DF GRASP orbitals.
TABLE I: Excitation energies (EE) and fine structure splitting (FS) (in cm\(^{-1}\)) of Mo VI and their comparison with experimental results. Contribution from absolute value of partial triple excitation to the EE (EE\(_{\text{triple}}\)) are also presented.

| State  | CC  | Exp.\(^a\) | CC  | Exp.\(^a\) | EE\(_{\text{triple}}\) |
|--------|-----|------------|-----|------------|------------------|
| 4d \(^2\)D\(_{3/2}\) | 0   | 0          | 0   | 0          | 0                |
| 4d \(^2\)D\(_{5/2}\) | 2670.55 | 2583.50  | 2670.55 | 2583.50 | 572.36           |
| 5s \(^2\)S\(_{1/2}\) | 118536.63 | 119725.62 | 396.72 |
| 5p \(^2\)P\(_{1/2}\) | 181795.01 | 182404.47 | 220.12 |
| 5p \(^2\)P\(_{3/2}\) | 186825.31 | 187331.19 | 5030.72 | 4926.72 | 235.92           |
| 4f \(^2\)F\(_{5/2}\) | 269411.28 | 267047.22 | 492.50 |
| 4f \(^2\)F\(_{7/2}\) | 269653.95 | 267456.84 | 242.67 | 409.62 | 621.98           |
| 5d \(^2\)D\(_{3/2}\) | 282598.52 | 282825.59 | 697.69 |
| 5d \(^2\)D\(_{5/2}\) | 283396.42 | 283610.94 | 797.90 | 785.35 | 816.42           |
| 6s \(^2\)S\(_{1/2}\) | 315632.41 | 313806.81 | 857.47 |
| 6p \(^2\)P\(_{1/2}\) | 342531.49 | 340570.78 | 690.67 |
| 6p \(^2\)P\(_{3/2}\) | 344853.69 | 342562.44 | 2322.21 | 1991.66 | 697.91 |

\(^a\) Ref. [15].

Pan and Beck [14]. Since, the contributions due to Breit interaction are relatively small, we do not consider them here self-consistently to evaluate wavefunctions.

Since the transition rate is proportional to the square of the transition amplitude, therefore precise description of the wavefunction is necessary due to one order higher dependence on wavefunctions than energy. In Table II, we compare the E1 transition amplitude in both length and velocity gauges for few transitions. We find a good agreement between them, which is one of the characteristics to judge the accuracy of the wavefunctions.

In Table III, we compare our \emph{ab initio} oscillator strength values correspond to E1 transitions with the recent semi-empirical calculations by Pan and Beck [14] and by Reader [15]. Reader has obtained wavefunctions using fitting parameters by comparing calculated and experimental energies, whereas, Pan and Beck have used relativistic CI method for the available transitions. Our calculated values of oscillator strength for the 4d \(^2\)D\(_{3/2}\) \(\rightarrow\) 4f \(^2\)F\(_{5/2}\)
TABLE II: Absolute values of E1 transition amplitude in length (D_l) and velocity (D_v) gauges for Mo VI.

| Term     | Upper  | Lower  | D_l  | D_v  |
|----------|--------|--------|------|------|
| 5p \(^2\)P_{1/2} \rightarrow 4d \(^2\)D_{3/2} | 0.9851 | 0.8341 |
| 5p \(^2\)P_{1/2} \rightarrow 5s \(^2\)S_{1/2} | 1.7554 | 1.7522 |
| 5p \(^2\)P_{3/2} \rightarrow 4d \(^2\)D_{3/2} | 0.4288 | 0.3619 |
| 5p \(^2\)P_{3/2} \rightarrow 5s \(^2\)S_{1/2} | 2.4885 | 2.5678 |
| 4f \(^2\)F_{5/2} \rightarrow 4d \(^2\)D_{3/2} | 1.3928 | 1.5438 |
| 4f \(^2\)F_{5/2} \rightarrow 4d \(^2\)D_{5/2} | 0.4272 | 0.4474 |
| 4f \(^2\)F_{7/2} \rightarrow 4d \(^2\)D_{5/2} | 2.6555 | 2.5330 |
| 5d \(^2\)D_{3/2} \rightarrow 5p \(^2\)P_{1/2} | 2.7486 | 2.6942 |
| 5d \(^2\)D_{3/2} \rightarrow 5p \(^2\)P_{3/2} | 1.2593 | 1.2278 |
| 5d \(^2\)D_{5/2} \rightarrow 5p \(^2\)P_{3/2} | 3.9600 | 3.7900 |
| 6s \(^2\)S_{1/2} \rightarrow 5p \(^2\)P_{1/2} | 0.9771 | 0.8873 |
| 6s \(^2\)S_{1/2} \rightarrow 5p \(^2\)P_{3/2} | 1.4711 | 1.1963 |
| 6p \(^2\)P_{1/2} \rightarrow 4d \(^2\)D_{3/2} | 0.1984 | 0.1686 |
| 6p \(^2\)P_{1/2} \rightarrow 5d \(^2\)D_{3/2} | 2.5559 | 2.2828 |
| 6p \(^2\)P_{1/2} \rightarrow 6s \(^2\)S_{1/2} | 3.4776 | 3.1844 |
| 6p \(^2\)P_{3/2} \rightarrow 4d \(^2\)D_{5/2} | 0.2845 | 0.2605 |
| 6p \(^2\)P_{3/2} \rightarrow 5d \(^2\)D_{3/2} | 1.1055 | 0.9949 |
| 6p \(^2\)P_{3/2} \rightarrow 6s \(^2\)S_{1/2} | 4.9149 | 4.6861 |

transition at the DF level given in the table, agrees well with similar calculations by Zilitis [13], 1.023.

Weighted oscillator strengths correspond to E1 transitions are presented in Table IV. Here we have used the length gauge values of E1 transition amplitudes and our calculated wavelengths. All these transitions, fall in ultraviolet and visible regions, are useful for astrophysical observations and may be for laboratory researches. According to Cowan [24], if the initial states are dominated by \(^2\)D and final states are dominated by \(^2\)P, the oscillator strength ratio of \(^2\)D_{5/2} \rightarrow \(^2\)P_{3/2}, \(^2\)D_{3/2} \rightarrow \(^2\)P_{1/2} and \(^2\)D_{3/2} \rightarrow \(^2\)P_{3/2} transitions in a given
TABLE III: Oscillator strengths for E1 transitions in length form and their comparison with earlier results.

| Term                        | Present calculations | Other calculations |
|-----------------------------|----------------------|--------------------|
|                             | Upper | Lower | DF | CC  | [15] | [14]  |
| $4d^2D_{3/2} \rightarrow 4f^2F_{5/2}$ | 1.0099| 0.3967| 0.3226| 0.2896|
| $4d^2D_{5/2} \rightarrow 4f^2F_{5/2}$ | 0.0484| 0.0246| 0.0153| 0.0139|

multiplet are 6:5:1, which we find the same for $4d^2D \rightarrow 5p^2P$ transitions.

In Table V, we present M1 and E2 transition probabilities and their corresponding wavelengths. However most of the transitions come in ultraviolet region, there are few transitions fall in infrared region. Though these transitions produce weak lines but they are important parameters in astrophysical studies. As expected, transition probability for E2 transitions come greater in value than that of M1 transitions except for the transitions fall in infrared region.

In Table VI, the contributions due to the different correlation terms like core-correlation, pair-correlation, core-polarization and important two-body contributions are estimated for few transitions to highlight the effect of correlations. Significant correlation contributions from the higher order core-polarization, like $S_{2f}^{(0,1)}O S_{2i}^{(0,1)}$, are noticeable compared to the lowest order contributions. Also, contributions from two-body correlations are almost comparable for most of the cases. For the M1 transition, $4d^2D_{5/2} \rightarrow 4d^2D_{3/2}$, there are cancelation observed among different correlation effects. The contribution comes from core-polarization term is more compared to other term. Even in the case of $5s^2S_{1/2} \rightarrow 4d^2D_{3/2}$ M1 transition, the Dirac-Fock contribution is almost canceled by the lowest order of core-polarization, which makes the core-corelation effect more dominant to the total value of transition matrix element.

Table VII summarizes the calculated lifetime of the low-lying excited states. Recent calculations of the lifetimes of $5p^2P_{1/2}$ and $5p^2P_{3/2}$ states by Zilitis [13] are also compared here. Here we can see that the lifetime of the $4d^2D_{5/2}$ state comes in the order of second, which suggest that Mo VI can be used for uniform doping in thin film. The lifetime of the $5s^2S_{1/2}$ state is found to be of the order of microsecond due to only forbidden transition contributions. Lifetime of the $5d$ states are larger than the $4f$ states due to strong contributions
TABLE IV: Transition wavelengths (in nm) and weighted oscillator strengths (gf) corresponding to electric dipole (E1) transitions of Mo VI.

| Term | Upper       | Lower       | $\lambda_{exp.}$ | gf   |
|------|-------------|-------------|------------------|------|
| 5p $^2P_{1/2} \rightarrow 4d^2D_{3/2}$ | 54.82 | 0.5354 |
| 5P $^2P_{1/2} \rightarrow 5s^2S_{1/2}$ | 159.54 | 0.5920 |
| 5p $^2P_{3/2} \rightarrow 4d^2D_{3/2}$ | 53.38 | 0.1042 |
| 5p $^2P_{3/2} \rightarrow 4d^2D_{5/2}$ | 54.12 | 0.9676 |
| 5p $^2P_{3/2} \rightarrow 5s^2S_{1/2}$ | 147.91 | 1.2844 |
| 4f $^2F_{5/2} \rightarrow 4d^2D_{3/2}$ | 37.44 | 1.5868 |
| 4f $^2F_{5/2} \rightarrow 4d^2D_{5/2}$ | 37.81 | 0.1478 |
| 4f $^2F_{7/2} \rightarrow 4d^2D_{5/2}$ | 37.75 | 5.7164 |
| 5d $^2D_{3/2} \rightarrow 5p^2P_{1/2}$ | 99.58 | 2.3133 |
| 5d $^2D_{3/2} \rightarrow 5p^2P_{3/2}$ | 104.71 | 0.4613 |
| 5d $^2D_{3/2} \rightarrow 4f^2F_{5/2}$ | 633.77 | 0.3446 |
| 5d $^2D_{5/2} \rightarrow 5p^2P_{3/2}$ | 103.86 | 4.5998 |
| 5d $^2D_{5/2} \rightarrow 4f^2F_{5/2}$ | 603.72 | 0.0260 |
| 5d $^2D_{5/2} \rightarrow 4f^2F_{7/2}$ | 619.03 | 0.5054 |
| 6s $^2S_{1/2} \rightarrow 5p^2P_{1/2}$ | 76.10 | 0.3881 |
| 6s $^2S_{1/2} \rightarrow 5p^2P_{3/2}$ | 79.06 | 0.8468 |
| 6p $^2P_{1/2} \rightarrow 4d^2D_{3/2}$ | 29.36 | 0.0409 |
| 6p $^2P_{1/2} \rightarrow 5s^2S_{1/2}$ | 44.87 | 0.0015 |
| 6p $^2P_{1/2} \rightarrow 5d^2D_{3/2}$ | 173.17 | 1.1894 |
| 6p $^2P_{1/2} \rightarrow 6s^2S_{1/2}$ | 373.63 | 0.9882 |
| 6p $^2P_{3/2} \rightarrow 4d^2D_{3/2}$ | 29.19 | 0.0092 |
| 6p $^2P_{3/2} \rightarrow 4d^2D_{5/2}$ | 29.41 | 0.0841 |
| 6p $^2P_{3/2} \rightarrow 5s^2S_{1/2}$ | 44.87 | 0.0559 |
| 6p $^2P_{3/2} \rightarrow 5d^2D_{3/2}$ | 167.40 | 0.2311 |
| 6p $^2P_{3/2} \rightarrow 5d^2D_{5/2}$ | 169.63 | 2.0902 |
| 6p $^2P_{3/2} \rightarrow 6s^2S_{1/2}$ | 347.75 | 2.1442 |
TABLE V: Transition wavelengths (in nm) and transition probabilities corresponding to electric quadrupole (E2) and magnetic dipole transitions (M1) (in sec\(^{-1}\)) of Mo VI.

| Term                  | Upper   | Lower   | \(\lambda_{exp.}\) | \(A_{E2}\)      | \(A_{M1}\)      |
|-----------------------|---------|---------|---------------------|-----------------|-----------------|
| 4d \(^2\)D\(_{5/2}\)/4d \(^2\)D\(_{3/2}\) | 3870.71 | 3.9372\(\times\)10\(^{-6}\) | 2.006\(\times\)10\(^{-1}\) |
| 5s \(^2\)S\(_{1/2}\)/4d \(^2\)D\(_{3/2}\) | 83.52   | 6.9919\(\times\)10\(^3\)  | 2.8677\(\times\)10\(^{-7}\) |
| 5s \(^2\)S\(_{1/2}\)/4d \(^2\)D\(_{5/2}\) | 85.36   | 9.3441\(\times\)10\(^3\)  |                        |
| 5p \(^2\)P\(_{3/2}\)/5p \(^2\)P\(_{1/2}\) | 2029.74 | 4.2402\(\times\)10\(^{-3}\) | 1.1401            |
| 4f \(^2\)F\(_{5/2}\)/5p \(^2\)P\(_{1/2}\) | 118.14  | 4.5388\(\times\)10\(^3\)  |                        |
| 4f \(^2\)F\(_{5/2}\)/5p \(^2\)P\(_{3/2}\) | 125.44  | 9.8580\(\times\)10\(^2\)  | 1.6191\(\times\)10\(^{-5}\) |
| 4f \(^2\)F\(_{7/2}\)/5p \(^2\)P\(_{3/2}\) | 124.80  | 4.2258\(\times\)10\(^3\)  |                        |
| 4f \(^2\)F\(_{7/2}\)/4f \(^2\)F\(_{5/2}\) | 24412.87| 7.5555\(\times\)10\(^{-11}\) | 1.3193\(\times\)10\(^{-4}\) |
| 5d \(^2\)D\(_{3/2}\)/4d \(^2\)D\(_{3/2}\) | 35.35   | 1.1221\(\times\)10\(^5\)  | 6.4795\(\times\)10\(^{-5}\) |
| 5d \(^2\)D\(_{3/2}\)/4d \(^2\)D\(_{5/2}\) | 35.68   | 4.8435\(\times\)10\(^4\)  | 2.8382\(\times\)10\(^1\)  |
| 5d \(^2\)D\(_{3/2}\)/5s \(^2\)S\(_{1/2}\) | 61.31   | 1.2090\(\times\)10\(^5\)  | 5.7627\(\times\)10\(^{-5}\) |
| 5d \(^2\)D\(_{5/2}\)/4d \(^2\)D\(_{3/2}\) | 35.25   | 3.1111\(\times\)10\(^4\)  | 2.5858            |
| 5d \(^2\)D\(_{5/2}\)/4d \(^2\)D\(_{5/2}\) | 35.58   | 1.2746\(\times\)10\(^5\)  | 1.6034\(\times\)10\(^1\)  |
| 5d \(^2\)D\(_{5/2}\)/5s \(^2\)S\(_{1/2}\) | 61.01   | 1.2112\(\times\)10\(^5\)  |                        |
| 5d \(^2\)D\(_{5/2}\)/5d \(^2\)D\(_{3/2}\) | 12733.17| 2.9790\(\times\)10\(^{-7}\) | 5.3860\(\times\)10\(^{-3}\) |
| 6s \(^2\)S\(_{1/2}\)/4d \(^2\)D\(_{3/2}\) | 31.86   | 1.7297\(\times\)10\(^2\)  | 1.5970\(\times\)10\(^{-3}\) |
| 6s \(^2\)S\(_{1/2}\)/4d \(^2\)D\(_{5/2}\) | 32.13   | 8.9836\(\times\)10\(^2\)  |                        |
| 6s \(^2\)S\(_{1/2}\)/5s \(^2\)S\(_{1/2}\) | 51.52   |                    | 2.9841            |
| 6s \(^2\)S\(_{1/2}\)/5d \(^2\)D\(_{3/2}\) | 322.77  | 2.6456\(\times\)10\(^2\)  | 2.6717\(\times\)10\(^{-6}\) |
| 6s \(^2\)S\(_{1/2}\)/5d \(^2\)D\(_{5/2}\) | 331.17  | 3.5638\(\times\)10\(^2\)  |                        |
| 6p \(^2\)P\(_{1/2}\)/5p \(^2\)P\(_{1/2}\) | 63.22   |                    | 8.4454\(\times\)10\(^{-2}\) |
| 6p \(^2\)P\(_{1/2}\)/5p \(^2\)P\(_{3/2}\) | 65.25   | 7.4911\(\times\)10\(^4\)  | 4.0073\(\times\)10\(^2\)  |
| 6p \(^2\)P\(_{1/2}\)/4f \(^2\)F\(_{5/2}\) | 136.01  |                    | 2.2749\(\times\)10\(^3\)  |
| 6p \(^2\)P\(_{3/2}\)/5p \(^2\)P\(_{1/2}\) | 62.44   | 3.6089\(\times\)10\(^4\)  | 1.3776\(\times\)10\(^2\)  |
| 6p \(^2\)P\(_{3/2}\)/5p \(^2\)P\(_{3/2}\) | 64.42   | 3.5807\(\times\)10\(^4\)  | 1.6161            |
| 6p \(^2\)P\(_{3/2}\)/4f \(^2\)F\(_{5/2}\) | 132.42  | 3.5357\(\times\)10\(^2\)  | 3.1526\(\times\)10\(^{-7}\) |
| 6p \(^2\)P\(_{3/2}\)/4f \(^2\)F\(_{7/2}\) | 131.34  | 2.0505\(\times\)10\(^3\)  |                        |
| 6p \(^2\)P\(_{3/2}\)/6p \(^2\)P\(_{1/2}\) | 5020.93 | 9.9619\(\times\)10\(^{-4}\) | 1.1185\(\times\)10\(^{-1}\) |
TABLE VI: Explicit contributions from the CCSD(T) calculations to the absolute magnitude of transition amplitudes.

| Dirac-Fock Core-corr. | Pair-corr. Core-polar. | Core-polar. Two-body Total (lowest) (higher) contr. |
|-----------------------|------------------------|--------------------------------------------------|
| 5p(1/2) → 4d(3/2) (E1) | -1.0898 -2.1536E-3 2.4778E-2 8.1783E-2 -3.1035E-2 -3.0657E-3 | -0.9851 |
| 5p(3/2) → 4d(3/2) (E1) | -0.4704 -8.5909E-4 1.1185E-2 3.1035E-2 -3.4575E-3 -3.1497E-3 | -0.4288 |
| 4d(5/2) → 4d(3/2) (E2) | 1.4451 -2.5900E-2 -3.1118E-2 -1.3272E-1 3.6817E-3 -1.1045E-3 | 1.2432 |
| 5s(1/2) → 4d(3/2) (E2) | 2.4193 2.8071E-3 -6.8921E-2 -3.1504E-2 2.1471E-2 -2.6223E-4 | 2.3176 |
| 4d(5/2) → 4d(3/2) (M1) | 1.5488 -1.3535E-2 -1.4813E-4 1.5097E-4 1.2398E-2 -1.8252E-3 | 1.5284 |
| 5s(1/2) → 4d(3/2) (M1) | -2.5086E-5 9.4303E-6 -3.1876E-7 2.4685E-5 -4.8217E-6 6.6800E-9 | 3.5805E-6 |

TABLE VII: Radiative lifetimes (in sec.) for different low-lying states of Mo VI.

| Term | Present calculations | Other calculations$^a$ |
|------|----------------------|-----------------------|
| 4d $^2D_{5/2}$ | 4.9854 | |
| 5s $^2S_{1/2}$ | 6.1213×10$^{-5}$ | |
| 5p $^2P_{1/2}$ | 1.4968×10$^{-10}$ | 1.300×10$^{-10}$ |
| 5p $^2P_{3/2}$ | 1.4151×10$^{-10}$ | 1.260×10$^{-10}$ |
| 4f $^2F_{5/2}$ | 7.1628×10$^{-11}$ | |
| 4f $^2F_{7/2}$ | 2.9462×10$^{-11}$ | |
| 5d $^2D_{3/2}$ | 2.1575×10$^{-10}$ | |
| 5d $^2D_{5/2}$ | 2.0922×10$^{-10}$ | |

$^a$ Ref. [13].

from the allowed dipole transitions 4f $^2F$ → 4d $^2D$.

IV. CONCLUSION

Forbidden transition probabilities among the low-lying states of Mo VI relevant for astro- and plasma physics are calculated using highly correlated relativistic coupled-cluster method for the first time in literature to the best of our knowledge. The lifetime of the 4d $^2D_{5/2}$ state is found to be around 5 second, which will be useful in many physical processes. Contributions of different correlation terms are discussed and found strong effect from higher order core-polarization. In the near future, present work will motivate experimentalists to verify our results due to its importance in many areas in physics.
V. ACKNOWLEDGMENT

We are grateful to Prof B P Das and Dr Rajat K Chaudhuri, Indian Institute of Astrophysics, Bangalore for providing the CC code. One of us (Narendra) would like to recognize the support of Council of Scientific and Industrial Research (CSIR), India.

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