

# Oscillator strengths and E1 radiative rates for Ca-like titanium, Ti III

A. A. El-maaref<sup>1,\*</sup>, Zaher Samak<sup>2</sup>, S. H. Allam<sup>2</sup> and Th. M. El-Sherbini<sup>2</sup>

<sup>1</sup>Physics Department, Faculty of Science, Al-Azhar University Assiut, 71524 Assiut, Egypt.

<sup>2</sup>Laboratory of Lasers and New Materials, Physics Department, Faculty of Science, Cairo University, Giza, Egypt.

Received: 20 Sep 2014, Revised: 16 Nov 2014, Accepted: 26 Nov 2014

Published online: 01 Jan 2015

**Abstract:** Configuration interaction calculations of oscillator strengths, transition probabilities, and lifetimes for transitions between levels belonging to calcium-like titanium (Ti III) have been executed using CIV3 code. A set of configuration state list of 220-configuration and correlations up to  $6l$  orbitals have been included in the calculations. The relativistic effects i.e, the Breit-Pauli Hamiltonian terms, such as the one body mass correction and Darwin term, and spin-orbit, spin-other-orbit, and spin-spin corrections, are included in the calculations. The present calculations of oscillator strengths are in good agreement with the published experimental and theoretical values.

**Keywords:** Energy levels; oscillator strengths; radiative rates, configuration interaction

## 1 Introduction

Iron group elements such as titanium and vanadium are of interest in astrophysics as well as plasma diagnostic. Many lines which appear in calcium-like titanium spectrum have been observed in the solar spectra, where lines of resonance array  $3d^2-3d4p$  have been identified [1]. The early work of atomic structure calculations for Ca-like Ti has been done by Warner and Kirkpatrick [2] based on the empirical derivation of Slater parameters. Experimentally, the oscillator strengths of Ti III have been measured using the wall-stabilized arc method [3]. Measurements of lifetimes by the beam foil technique and branching ratio using the wall-stabilized arc method have been used to determine the oscillator strengths of Ti II and lifetimes of Ti III [4]. Fuhr et. al. [5] have compiled experimental and theoretical data of oscillator strengths and transition probabilities for iron through nickel including Ti III. Morton and Smith [6] have prepared a compilation of experimental and theoretical values of oscillator strengths, wavelengths and excitation energies of 499 atomic spectral lines including calcium-like titanium. Recently, Raassen and Uylings [7] have calculated transition probabilities of iron group ions Ti III and V IV using the orthogonal operators method. Zhang et.al. [8] have calculated oscillator strengths and

transition probabilities of Ti III and V IV using the Weakest Bound Electron Potential Model (WBEPM) theory.

From the perspective that there are no adequate studies cover the need of atomic data of Ca-like titanium, we offer this work to complement the few previous studies related to this ion under consideration. In the present work, configuration interaction calculations of oscillator strengths and electronic dipole transition rates have been performed for calcium-like titanium using CIV3 code [9]. A set of 220 configurations has been used in the calculations, and the relativistic correlations by including the Breit-Pauli Hamiltonian as well as the correlations up to  $6l$  orbitals have been included within the calculations. The convergence between  $f_L$  and  $f_V$  values gives a strong indicator of the calculations accuracy. Moreover, the present work provide spectroscopic results for excited levels in heavy atoms, which are applicable in the fields of plasma physics, astrophysics, and controlled thermonuclear fusion [10].

## 2 Method of calculation

The present calculations have been performed using the configuration interaction method (CIV3 code), which

\* Corresponding author e-mail: [aahmh@hotmail.com](mailto:aahmh@hotmail.com)

includes relativistic correlations (Breit-Pauli Hamiltonian) [9,11]. The  $LS$  states belonging to configurations of Ca-like Ti III give about of 151 transitions between levels corresponding to various  $J$  values. All  $LS$  states considered here are expressed as linear combinations of configurational wavefunctions in the form:

$$\Psi(L,S) = \sum_i^M a_{i,LS} \phi_i[\alpha_i LS] \quad (1)$$

The single configuration wavefunctions  $\phi_i$  are built from one electron functions (orbitals) whose angular momenta are coupled in a manner defined by  $\alpha_{i,LS}$ , to form a total  $L$  and  $S$  common to all configurations in Eq 1. Thus the functions  $\phi_i$  are eigenfunctions of  $L^2$  and  $S^2$ . Each one electron orbital is a product of a radial function, a spherical harmonic and a spin function of the form:

$$u(r, m_s) = r^{-1} P_{nl}(r) Y_l(\theta, \varphi) \chi(m_s) \quad (2)$$

with  $\int_0^\infty P_{nl}(r) P_{ml}(r) dr = \delta_{nm}; l+1 < m \leq n$ .

The radial functions  $P_{nl}(r)$  can be expanded analytically as sums of normalized Slater type orbitals

$$P_{nl}(r) = \sum_{i=1}^k C_i N_i r^{p_i} \exp(-\xi_i r) \quad (3)$$

where

$$N_i = \left( \frac{2(\xi_i)^{2p_i+1}}{(2p_i)!} \right). \quad (4)$$

In Eq 3, for each orbital, the powers of  $r$  (the  $p_i$ ) are kept fixed and the coefficients  $C_i$ , and  $\xi_i$  are the exponents of the normalized Slater type orbitals, which treated as variational parameters. The  $J$ -dependent configuration interactions expansion takes the form [12]:

$$\Psi_i(JM_J) = \sum_{j=1}^K b_{ij} \phi_j(\alpha_j L_j S_j J M_J) \quad (5)$$

where  $\phi_j$  denotes a set of configurational wavefunctions each describe single configuration,  $\alpha_j$  defines the  $LS$  coupling of the electrons and  $J = L + S$ . The mixing parameters ( $b_{ij}$ ) are calculated by diagonalizing the Breit-Pauli Hamiltonian matrix relative to a set of single-configuration wavefunctions ( $\phi_j$ ). The fine structure energy levels, oscillator strengths and transition probabilities have been calculated by using the wavefunctions in Eq 5.

In the present work, we have used the 1s, 2s, 2p, 3s,3p and 3d radial functions as the Hartree-Fock orbitals of the ground state  $3p^6 3d^2$  of Ca-like titanium as they given in Ref. [13]. While the other radial functions for the 4l, 5s, 5p, 5d, and 5f orbitals are chosen as a spectroscopic. The radial wavefunctions of the spectroscopic orbitals have been optimized using the CIV3 program [10]. The 6s-6f orbitals are chosen as a correlation orbitals. Table 1 shows the radial parameters which have been used in the calculations.

**Table 1:** Radial function parameters for optimized orbitals of Ca-like Ti III.

$nl$	$p_i$	Exponents- $\xi_i$
4s	1	22.946790
	2	8.567990
	3	1.959588
	4	1.545990
4p	2	1.730011
	3	9.899990
	4	3.999900
	4	0.588750
4d	4	1.334690
	4	0.393320
4f	4	0.393320
	4	0.393320
5s	1	29.900000
	2	7.999990
	3	3.999990
	4	1.750000
	5	1.009990
5p	2	0.769790
	3	2.389870
	4	0.479500
	5	3.758010
	5	1.999900
5d	3	2.253550
	4	2.888600
	5	1.999900
5f	4	0.394750
	5	0.298990
	5	0.298990
6s	1	2.989990
	2	1.081990
	3	0.801660
	4	2.190000
	5	1.009990
	6	0.979990
6p	2	2.840000
	3	1.000000
	4	1.000000
	5	13.999990
	6	2.799999
6d	3	5.989950
	4	3.112466
	5	1.120030
	6	0.689990
6f	4	0.121250
	5	0.099900
	6	0.502630

The coefficients  $C_i$  are already computed by the orthogonality condition on  $P_{nl}$  within the code and the parameter  $k = n - l$  has been taken in Eq 3. Finally, the Hamiltonian of the whole atom or ion can be represented by the non-relativistic electrostatic interaction in addition to the Breit-Pauli Hamiltonian which consists of: one body mass correction, Darwin term, spin-orbit, spin-other-orbit and spin-spin operator [14]. The oscillator strengths in length and velocity gauge forms are given by [15]:

$$f_{ij}^L = [2\Delta E/3] |\langle \psi_j | r | \psi_i \rangle|^2 \quad (6)$$

$$f_{ij}^V = [2/3\Delta E]|\langle\psi_j|\nabla|\psi_i\rangle|^2 \quad (7)$$

### 3 Results and Discussion

#### 3.1 Oscillator strengths

We exclude the data of level energies from this study, because we think that we cannot offer any significant new results. There are 200 energy levels have been published in the NIST atomic database spectra [16], but we have included in table 3 values of wavelengths (in Å) of 151 electronic dipole transition between levels belonging to Ca-like titanium. The present CIV3 calculations of oscillator strengths in both length ( $f_L$ ) and velocity ( $f_V$ ) forms have been listed in table 3. It can be seen that most of our results agree well with those taken from the NIST database [16] for most transitions the deviations between our values and NIST values better than 25%, but in a few cases the relative differences reach to 46, 58% such as transitions numbers 5 and 10 in table 3, respectively. This worse agreement might due to the limited number of configurations which used in the calculation process. Actually, the NIST values are a compilation of experimental and theoretical data from previous works [17,18,19], and the estimated accuracies of most oscillator strengths and transition probabilities recorded in the NIST database [16] are quoted to be between 40 and 50%. Another work we have used to compare our results with it is the study by Zhang et.al. [8] which presented oscillator strengths and transition probabilities of Ti III, they focused their calculations on the transitions between high-lying levels (4*l*, 5*l*, and 6*l*). When comparison is available, our calculations show good agreements with those in Ref [8].

The precision of the theoretical calculations can be judged by the convergence between length and velocity gauge values of oscillator strengths. If exact wave functions are used then  $f_L = f_V$ . Which is convincingly fulfilled in the most of our calculations, where the value  $f_L/f_V$  approximately equal unit for most of our transitions. In some cases the difference between  $f_L$  and  $f_V$  reach to large values, for instance, transitions 118; 3d4d ( $^3F_4$ )- 3d5f ( $^3G_3$ ), 119; 3d4d ( $^3F_4$ )- 3d5f ( $^3G_4$ ), and 120; 3d4d ( $^3F_4$ )- 3d5f ( $^3G_5$ ). These large differences between  $f_L$  and  $f_V$  might be due to a higher correlations up to  $nl > 6l$  should be included in the calculations. For allowed transitions, the transition operator is expressed in the length form, where the relativistic corrections are automatically included, as well as additional terms should be incorporated to the gradient matrix elements to keep the equivalence between length and velocity forms [20]. In cases where the *LS* coupling scheme is sufficiently good, the velocity form (uncorrected gradient) could still be used for allowed transitions, even when calculated in the Breit-Pauli approximation, in the length-velocity

agreement as a quality and convergence criterion. But, even in these cases, it must be borne in mind that the results are not strictly valid. For spin-forbidden transitions, the velocity form is unsuitable [21].

#### 3.2 Radiative rates

The present calculations of transition probabilities  $A_L$  (in  $s^{-1}$ ) are listed in table 3. Table 2 contains values of lifetimes for some excited levels in Ca-like Ti III. The lifetimes of excited levels can be calculated from [22]:

$$\tau_j = \frac{1}{\sum_i A_{ji}} \quad (8)$$

where the sum over *i* is over all accessible final states and  $\Delta E = E_j - E_i$ . Unfortunately, only a few values of lifetimes are available to compare our data with it in Ref [4]. The calculated lifetime show a reasonable agreement with the few available values by Roberts et al [4]. Actually, the accuracy of energies reflect on the precision of wavelengths and transition rates, hence, to get high accuracy in the case of a heavy atoms such as titanium a higher contribution should be expected from the similar levels [23] which are fulfilled by adding up to 6*f* correlations.

### 4 Conclusion

In this study, oscillator strengths and allowed transition probabilities for Ca-like titanium (Ti III) have been calculated using the CIV3 code. Our calculated results show a good agreement with previous works, as well as with the values from the NIST Atomic Spectra Database. The present results might be useful in thermonuclear fusion researches, astrophysical applications and technical plasma modeling.

**Table 2:** Lifetimes (in ns) of some exited levels in calcium-like titanium.

Configuration	$\tau$ (present)	$\tau$ Ref. [4]	Configuration	$\tau$ (present)	$\tau$ Ref. [4]
3d4p ( $^1D_2$ )	1.93	2.7	3d4p ( $^1F_3$ )	–	1.4
3d4p ( $^3D_3$ )	1.65	1.7	3d4p ( $^3F_2$ )	2.48	2.6
3d4p ( $^3D_1$ )	0.475		3d4p ( $^3F_4$ )	4.51	
3d4p ( $^3D_2$ )	1.13		3d4f ( $^3F_2$ )	125	
3d4p ( $^1P_1$ )	–	2.3	3d4f ( $^3F_3$ )	3.13	
3d4d ( $^3F_2$ )	1.37		3d4f ( $^3F_4$ )	1.90	
3d4d ( $^3F_3$ )	1.58		3d4f ( $^3G_3$ )	13.90	
3d4d ( $^3F_3$ )	1.62		3d4f ( $^3G_4$ )	2.87	
3d4d ( $^3P_1$ )	9.30		3d4f ( $^3G_5$ )	0.597	
3d4d ( $^3P_1$ )	8.27		3d4f ( $^3D_2$ )	9.21	
3d4d ( $^3S_1$ )	1470		3d4d ( $^3D_2$ )	3.11	
3d4d ( $^1P_1$ )	5.06		3d4d ( $^3D_3$ )	4.00	

## References

- [1] S.O. Kastner, *Solar Physics*, **151**, 41-49 (1994).
- [2] B. Warner and C. Kirkpatrick, *Monthly Notices of the Royal Astronomical Society*, **144**, 397-410 (1969).
- [3] J.R. Roberts and P.A. Voigt, *The Astrophysical Journal*, **197**, 791-798 (1975).
- [4] J.R. Roberts, T. Andersen and G. Sorensen, *The Astrophysical Journal*, **181**, 567-586 (1973).
- [5] J.R. Fuhr, G.A. Martin, and W.L. Wise, *Journal Physical and Chemical Reference Data*, **17**, 1-499 (1988).
- [6] D.C. Morton and W.H. Smith, *The Astrophysical Journal*, **233**, 333-363 (1973).
- [7] A.J.J. Raassen and P.H.M. Uylings, *Astronomy and Astrophysical Supplement Series*, **123**, 147-158 (1997).
- [8] T. Zhang, N. Zhang, and D. Ma, *International Journal of Quantum Chemistry*, **109**, 145-159 (2009).
- [9] A. Hibbert, *Computer Physics Communications*, **9**, 141-172 (1975).
- [10] A. Abou El-Maaref, S.H. Allam and Th.M. El-Sherbini, *Atomic Data and Nuclear Data Tables*, **100**, 155-182 (2014).
- [11] R. Glass and A. Hibbert, *Computer Physics Communications*, **11**, 125-140 (1976).
- [12] R. Glass and A. Hibbert, *Computer Physics Communications*, **16**, 19-34 (1978).
- [13] E. Clementi and C. Roetti, *Atomic Data and Nuclear Data Tables*, **14**, 177-478 (1974).
- [14] V. Tayal and G.P. Gupta, *Physica Scripta*, **75**, 331-339 (2007).
- [15] A. Hibbert, Atomic structure theory in Progress in Atomic Spectroscopy (eds.) W. Hanle and H. Kleinpoppen (New York : Plenum) pp1(1979).
- [16] NIST Atomic Database Spectra: <http://physics.nist.gov/cgi-bin/ASD/energy1.pl>.
- [17] B. Warner and R. C. Kirkpatrick, Publ. Dept. Astron. Univ. Texas, Austin 3(2), 1-318 (1969).
- [18] T. Shirai, J. Sugar, A. Musgrove, and W. L. Wiese, AIP Press, Melville, NY, 1-632 (2000).
- [19] R.L. Kurucz and E. Peytremann, Smithsonian Astrophysical Observatory Special Report 362 (Cambridge, Mass., 1975).
- [20] W. F. Drake, *Journal of Physics B*, **9**, L169 (1976).
- [21] G.P. Gupta and A.Z. Msezane, *Atomic Data and Nuclear Data Tables*, **74**, 267-282 (2000).
- [22] A. Hibbert, *Reports on Progress in Physics*, **38**, 1217-1338 (1975).
- [23] Th.M. El-Sherbini, *Journal of Physics B*, **9**, 1665 (1976).

**Table 3:** Wavelengths in Å, oscillator strengths and transition probabilities (in s<sup>-1</sup>) of Ca-like Ti. LL. indicates lower levels and UL. indicates upper levels.

Index	UL.	LL.	$\lambda$	$f_L$	$f_V$	$A_L$	$f$ Ref.[8]	$f_{NIST}$
1	3d 4p ( <sup>3</sup> D <sub>3</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>2</sub> )	1291.25	2.19E-03	1.86E-03	6.26E+06		
2	3d 4p( <sup>3</sup> F <sub>3</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>2</sub> )	1288.54	2.94E-03	2.20E-02	8.44E+06		
3	3d 4p( <sup>1</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>2</sub> )	1328.81	7.78E-05	6.98E-05	2.94E+05		
4	3d 4p( <sup>3</sup> D <sub>1</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>2</sub> )	1293.85	9.94E-02	8.44E-02	6.60E+08		
5	3d 4p( <sup>3</sup> F <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>2</sub> )	1290.90	3.20E-02	2.23E-02	1.28E+09		6.0E-02
6	3d 5p( <sup>3</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>2</sub> )	1292.02	1.84E-02	1.55E-02	7.34E+07		
7	3d 4p( <sup>1</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>3</sub> )	1332.05	4.44E-04	4.00E-04	2.34E+06		
8	3d 4p ( <sup>3</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>3</sub> )	1296.23	8.32E-02	7.09E-02	4.62E+08		8.9E-02
9	3d 4p ( <sup>3</sup> D <sub>3</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>3</sub> )	1294.31	9.03E-03	7.69E-03	3.60E+07		
10	3d 4p( <sup>3</sup> F <sub>3</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>3</sub> )	1291.58	2.30E-02	1.56E-02	9.21E+07		5.5E-02
11	3d 4p( <sup>3</sup> D <sub>3</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>3</sub> )	1298.34	7.28E-02	6.23E-02	3.70E+08		
12	3d 5p( <sup>3</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>3</sub> )	1295.08	1.05E-01	8.91E-02	5.83E+08		
13	3d 4p( <sup>3</sup> F <sub>4</sub> )	3d <sup>2</sup> ( <sup>3</sup> F <sub>4</sub> )	1294.76	5.57E-02	4.75E-02	2.22E+08		5.0E-02
14	3d 4p( <sup>3</sup> P <sub>1</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>0</sub> )	1417.44	1.29E-01	1.16E-01	1.43E+08		1.10E-01
15	3d 4p( <sup>1</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>1</sub> )	1546.22	1.28E-04	1.41E-04	2.13E+05		
16	3d 4p( <sup>3</sup> D <sub>1</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>1</sub> )	1499.09	1.01E-02	1.05E-02	3.00E+07		
17	3d 4p( <sup>3</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>1</sub> )	1498.17	1.70E-02	1.76E-02	3.04E+07		
18	3d 4p( <sup>3</sup> F <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>1</sub> )	1495.12	7.11E-05	1.85E-04	1.27E+05		
19	3d 4p( <sup>3</sup> P <sub>0</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>1</sub> )	1420.74	4.30E-02	3.89E-02	4.26E+08		4.0E-02
20	3d 4p( <sup>3</sup> P <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>1</sub> )	1414.32	5.40E-02	4.84E-02	1.08E+08		4.50E-02
21	3d 4p( <sup>3</sup> D <sub>3</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>2</sub> )	1498.39	1.43E-02	1.48E-02	3.03E+07		2.3E-02
22	3d 4p( <sup>3</sup> F <sub>3</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>2</sub> )	1494.74	1.04E-04	2.70E-04	2.21E+05		
23	3d 4p( <sup>1</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>2</sub> )	1549.20	4.17E-05	1.58E-05	1.16E+05		
24	3d 4p( <sup>3</sup> D <sub>1</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>2</sub> )	1501.89	4.00E-04	4.16E-04	1.97E+06		
25	3d 4p( <sup>3</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>2</sub> )	1500.97	3.37E-03	3.50E-03	9.98E+06		
26	3d 4p( <sup>3</sup> F <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>2</sub> )	1497.92	1.41E-05	3.67E-05	4.18E+04		
27	3d 4p( <sup>3</sup> P <sub>2</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>2</sub> )	1416.82	9.61E-02	8.66E-02	3.19E+08		9.1E-02
28	3d 4p( <sup>3</sup> P <sub>1</sub> )	3d <sup>2</sup> ( <sup>3</sup> P <sub>2</sub> )	1421.20	3.19E-02	2.89E-02	1.76E+08		2.9E-02
29	3d 4p( <sup>3</sup> D <sub>3</sub> )	3d <sup>2</sup> ( <sup>1</sup> D <sub>2</sub> )	1456.40	1.31E-04	1.28E-04	2.94E+05		
30	3d 4p( <sup>1</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>1</sup> D <sub>2</sub> )	1504.35	9.24E-02	9.89E-02	2.72E+08		9.40E-02
31	3d 4p( <sup>1</sup> P <sub>1</sub> )	3d <sup>2</sup> ( <sup>1</sup> D <sub>2</sub> )	1383.36	5.62E-04	4.76E-04	3.26E+06		
32	3d 4p( <sup>1</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>1</sup> D <sub>2</sub> )	1504.35	9.24E-02	9.89E-02	2.72E+08		9.40E-02
33	3d 4p( <sup>3</sup> D <sub>1</sub> )	3d <sup>2</sup> ( <sup>1</sup> D <sub>2</sub> )	1459.70	3.67E-06	3.60E-06	1.92E+04		
34	3d 4p( <sup>3</sup> D <sub>2</sub> )	3d <sup>2</sup> ( <sup>1</sup> D <sub>2</sub> )	1458.83	3.10E-05	3.03E-05	9.71E+04		
35	3d 4p( <sup>3</sup> F <sub>2</sub> )	3d <sup>2</sup> ( <sup>1</sup> D <sub>2</sub> )	1455.95	1.32E-07	3.19E-07	4.15E+02		
36	3d 4p( <sup>3</sup> D <sub>3</sub> )	3d <sup>2</sup> ( <sup>1</sup> G <sub>4</sub> )	1577.45	5.99E-09	5.78E-09	2.06E+01		
37	3d 4p( <sup>3</sup> F <sub>3</sub> )	3d <sup>2</sup> ( <sup>1</sup> G <sub>4</sub> )	1573.40	4.42E-09	4.24E-09	1.53E+01		
38	3d 4p( <sup>1</sup> F <sub>3</sub> )	3d <sup>2</sup> ( <sup>1</sup> G <sub>4</sub> )	1424.21	1.50E-01	1.66E-01	6.36E+08		1.6E-01
39	3d 4p( <sup>1</sup> D <sub>2</sub> )	3d 4s( <sup>1</sup> D <sub>2</sub> )	2959.85	3.15E-01	2.32E-01	2.40E+08	2.75E-01	2.50E-01
40	3d 4p ( <sup>3</sup> F <sub>2</sub> )	3d 4s ( <sup>3</sup> D <sub>2</sub> )	2545.12	5.19E-02	6.63E-02	5.35E+07		
41	3d 5p ( <sup>3</sup> F <sub>2</sub> )	3d 4s ( <sup>3</sup> D <sub>3</sub> )	917.00	9.04E-06	1.29E-05	1.00E+05		
42	3d 5p ( <sup>3</sup> F <sub>3</sub> )	3d 4s ( <sup>3</sup> D <sub>3</sub> )	915.80	3.54E-04	3.31E-04	2.82E+06		
43	3d 4p ( <sup>1</sup> D <sub>2</sub> )	3d 4s ( <sup>3</sup> D <sub>3</sub> )	2711.01	1.64E-04	1.11E-04	2.09E+05		
44	3d 4d( <sup>3</sup> F <sub>2</sub> )	3d 4p( <sup>1</sup> D <sub>2</sub> )	1715.93	1.89E-04	1.97E-04	4.28E+05		
45	3d 4d( <sup>3</sup> F <sub>3</sub> )	3d 4p( <sup>1</sup> D <sub>2</sub> )	1713.04	1.51E-03	1.57E-03	2.46E+06		
46	3d 4d( <sup>3</sup> P <sub>1</sub> )	3d 4p( <sup>1</sup> D <sub>2</sub> )	1676.74	2.03E-04	2.01E-04	8.04E+05		
47	3d 4d( <sup>1</sup> D <sub>2</sub> )	3d 4p( <sup>1</sup> D <sub>2</sub> )	1690.41	2.30E-01	2.37E-01	5.37E+08		
48	3d 4d( <sup>3</sup> P <sub>2</sub> )	3d 4p( <sup>1</sup> D <sub>2</sub> )	1674.45	1.13E-03	1.51E-03	2.69E+06		
49	3d 4d( <sup>3</sup> P <sub>2</sub> )	3d 4p( <sup>3</sup> D <sub>1</sub> )	1733.47	1.63E-03	1.72E-03	2.17E+06		
50	3d 4d ( <sup>1</sup> P <sub>2</sub> )	3d 4p ( <sup>1</sup> D <sub>2</sub> )	1814.92	5.86E-02	6.86E-02	1.98E+08		
51	3d 4d ( <sup>3</sup> S <sub>1</sub> )	3d 4p ( <sup>1</sup> D <sub>2</sub> )	1787.43	2.01E-04	2.79E-04	6.98E+05		
52	3d 4d ( <sup>3</sup> D <sub>2</sub> )	3d 4p ( <sup>1</sup> D <sub>2</sub> )	1832.62	7.12E-04	8.34E-04	1.42E+06		
53	3d 4d( <sup>3</sup> F <sub>2</sub> )	3d 4p( <sup>3</sup> D <sub>1</sub> )	1777.97	3.79E-01	4.23E-01	4.80E+08		
54	3d 4d( <sup>1</sup> D <sub>2</sub> )	3d 4p( <sup>3</sup> D <sub>1</sub> )	1750.58	4.89E-05	5.26E-05	6.39E+04		
55	3d 4d ( <sup>3</sup> P <sub>2</sub> )	3d 4p ( <sup>3</sup> D <sub>1</sub> )	1903.55	5.70E-02	7.19E-02	6.30E+07	2.01E-03	

Table 3 – continued

Index	UL.	LL.	$\lambda$	$f_L$	$f_V$	$A_L$	$f$ Ref.[8]	$f_{NIST}$
56	3d 4d( <sup>1</sup> D <sub>2</sub> )	3d 4p( <sup>3</sup> D <sub>2</sub> )	1751.83	2.47E-04	2.66E-04	5.37E+05		
57	3d 4d( <sup>3</sup> P <sub>2</sub> )	3d 4p( <sup>3</sup> D <sub>2</sub> )	1734.70	8.25E-03	8.71E-03	1.83E+07		
58	3d 4d( <sup>3</sup> F <sub>2</sub> )	3d 4p( <sup>3</sup> D <sub>2</sub> )	1779.27	5.68E-03	6.37E-03	1.19E+07		
59	3d 4d( <sup>3</sup> F <sub>3</sub> )	3d 4p( <sup>3</sup> D <sub>2</sub> )	1776.16	2.67E-01	2.97E-01	4.03E+08		
60	3d 4d( <sup>3</sup> P <sub>1</sub> )	3d 4p( <sup>3</sup> D <sub>2</sub> )	1737.16	2.55E-02	2.70E-02	9.38E+07		
61	3d 4d( <sup>3</sup> D <sub>2</sub> )	3d 4p( <sup>3</sup> D <sub>2</sub> )	1905.04	1.11E-01	1.41E-01	2.05E+08		
62	3d 4d( <sup>3</sup> D <sub>3</sub> )	3d 4p( <sup>3</sup> D <sub>2</sub> )	1901.45	2.17E-02	2.73E-02	2.86E+07		
63	3d 4d( <sup>3</sup> G <sub>3</sub> )	3d 4p( <sup>3</sup> D <sub>2</sub> )	1894.04	2.19E-01	2.74E-01	2.91E+08		
64	3d 4d( <sup>3</sup> F <sub>4</sub> )	3d 4p( <sup>3</sup> D <sub>3</sub> )	1775.64	2.15E-01	2.39E-01	3.53E+08		
65	3d 4d( <sup>3</sup> F <sub>2</sub> )	3d 4p( <sup>3</sup> D <sub>3</sub> )	1782.90	3.53E-03	3.97E-03	1.04E+07		
66	3d 4d( <sup>3</sup> F <sub>3</sub> )	3d 4p( <sup>3</sup> D <sub>3</sub> )	1779.78	2.03E-02	2.28E-02	4.28E+07		
67	3d 4d( <sup>1</sup> D <sub>2</sub> )	3d 4p( <sup>3</sup> D <sub>3</sub> )	1755.36	7.44E-04	8.05E-04	2.25E+06		
68	3d 4d( <sup>3</sup> P <sub>2</sub> )	3d 4p( <sup>3</sup> D <sub>3</sub> )	1738.15	2.48E-02	2.63E-02	7.67E+07		
69	3d 4d( <sup>1</sup> G <sub>4</sub> )	3d 4p( <sup>3</sup> D <sub>3</sub> )	1485.78	1.67E-09	2.15E-10	3.93E+00		
70	3d 4d( <sup>3</sup> D <sub>2</sub> )	3d 4p( <sup>3</sup> D <sub>3</sub> )	1909.20	3.72E-05	4.62E-05	9.53E+04		
71	3d 4d( <sup>3</sup> D <sub>3</sub> )	3d 4p( <sup>3</sup> D <sub>3</sub> )	1905.60	1.07E-01	1.35E-01	1.97E+08		
72	3d 4d( <sup>3</sup> G <sub>4</sub> )	3d 4p( <sup>3</sup> D <sub>3</sub> )	1893.41	2.70E-01	3.37E-01	3.91E+08		
73	3d 4d( <sup>3</sup> G <sub>3</sub> )	3d 4p( <sup>3</sup> D <sub>3</sub> )	1898.16	1.80E-02	2.26E-02	3.33E+07		
74	3d 4d( <sup>3</sup> P <sub>2</sub> )	3d 4p( <sup>3</sup> F <sub>2</sub> )	1738.80	1.15E-03	1.62E-04	2.53E+06		
75	3d 4d( <sup>3</sup> F <sub>2</sub> )	3d 4p( <sup>3</sup> F <sub>2</sub> )	1783.58	9.95E-02	8.76E-02	2.09E+08	1.56E-01	
76	3d 4d( <sup>3</sup> D <sub>3</sub> )	3d 4p( <sup>3</sup> F <sub>2</sub> )	1906.37	1.94E-03	1.52E-03	2.54E+06		
77	3d 4d( <sup>3</sup> G <sub>3</sub> )	3d 4p( <sup>3</sup> F <sub>2</sub> )	1898.92	2.81E-01	3.52E-01	3.71E+08		
78	3d 4d( <sup>3</sup> F <sub>2</sub> )	3d 4p( <sup>3</sup> F <sub>3</sub> )	1788.10	5.83E-03	5.60E-03	1.70E+07		
79	3d 4d( <sup>3</sup> F <sub>3</sub> )	3d 4p( <sup>3</sup> F <sub>3</sub> )	1784.96	7.47E-02	6.38E-02	1.56E+08	1.48E-01	
80	3d 4d( <sup>3</sup> P <sub>2</sub> )	3d 4p( <sup>3</sup> F <sub>3</sub> )	1743.09	6.02E-03	8.53E-04	1.85E+07		
81	3d 4d( <sup>1</sup> G <sub>4</sub> )	3d 4p( <sup>3</sup> F <sub>3</sub> )	1489.38	1.23E-09	1.59E-10	2.87E+00		
82	3d 4d( <sup>3</sup> D <sub>2</sub> )	3d 4p( <sup>3</sup> F <sub>3</sub> )	1915.17	1.76E-02	1.29E-02	4.47E+07		
83	3d 4d( <sup>3</sup> D <sub>3</sub> )	3d 4p( <sup>3</sup> F <sub>3</sub> )	1911.54	1.20E-02	4.65E-04	2.19E+07		
84	3d 4d( <sup>3</sup> G <sub>3</sub> )	3d 4p( <sup>3</sup> F <sub>3</sub> )	1904.05	1.32E-02	1.66E-02	2.43E+07		
85	3d 4d( <sup>3</sup> G <sub>4</sub> )	3d 4p( <sup>3</sup> F <sub>3</sub> )	1899.27	1.98E-01	2.49E-01	2.85E+08		
86	3d 5d( <sup>1</sup> D <sub>2</sub> )	3d 4p( <sup>3</sup> F <sub>3</sub> )	1048.34	5.37E-05	4.64E-06	4.56E+05		
87	3d 4d( <sup>3</sup> F <sub>4</sub> )	3d 4p( <sup>3</sup> F <sub>4</sub> )	1782.39	1.26E-01	1.42E-01	2.65E+08		
88	3d 4d( <sup>3</sup> F <sub>3</sub> )	3d 4p( <sup>3</sup> F <sub>4</sub> )	1786.56	8.39E-03	9.47E-03	2.25E+07	1.10E-02	
89	3d 4d( <sup>3</sup> S <sub>1</sub> )	3d 4p( <sup>3</sup> P <sub>0</sub> )	1990.66	1.25E-01	1.65E-01	7.02E+07		2.2E-01
90	3d 4d( <sup>3</sup> D <sub>1</sub> )	3d 4p( <sup>3</sup> P <sub>0</sub> )	2049.65	2.20E-01	3.10E-01	1.16E+08		3.4E-01
91	3d 4d( <sup>3</sup> D <sub>1</sub> )	3d 4p( <sup>3</sup> P <sub>1</sub> )	2053.94	5.48E-02	7.75E-02	8.66E+07	8.18E-02	7.30E-02
92	3d 4d( <sup>3</sup> D <sub>2</sub> )	3d 4p( <sup>3</sup> P <sub>1</sub> )	2051.16	1.65E-01	2.32E-01	1.57E+08	2.46E-01	2.80E-01
93	3d 4d( <sup>3</sup> S <sub>1</sub> )	3d 4p( <sup>3</sup> P <sub>1</sub> )	1994.72	1.24E-01	1.65E-01	2.08E+08	2.46E-01	2.1E-01
94	3d 4d( <sup>3</sup> S <sub>1</sub> )	3d 4p( <sup>3</sup> P <sub>2</sub> )	2003.40	1.24E-01	1.66E-01	3.45E+08		2.0E-01
95	3d 4d( <sup>3</sup> D <sub>3</sub> )	3d 4p( <sup>3</sup> P <sub>2</sub> )	2056.16	1.84E-01	2.61E-01	2.07E+08		3.00E-01
96	3d 4d( <sup>3</sup> D <sub>2</sub> )	3d 4p( <sup>3</sup> P <sub>2</sub> )	2060.35	3.28E-02	4.67E-02	5.15E+07	4.91E-02	3.70E-02
97	3d 5p( <sup>3</sup> D <sub>2</sub> )	3d 4d( <sup>3</sup> F <sub>2</sub> )	1781.45	4.18E-02	4.69E-02	8.79E+07		
98	3d 5p( <sup>3</sup> F <sub>2</sub> )	3d 4d( <sup>3</sup> F <sub>2</sub> )	1783.58	9.95E-02	8.76E-02	2.09E+08		
99	3d 5f( <sup>3</sup> F <sub>2</sub> )	3d 4d( <sup>3</sup> F <sub>2</sub> )	1997.27	1.17E-01	1.80E-02	1.95E+08		
100	3d 5p( <sup>3</sup> D <sub>2</sub> )	3d 4d( <sup>3</sup> F <sub>3</sub> )	1778.33	3.35E-01	3.74E-01	5.05E+08		
101	3d 5p( <sup>3</sup> D <sub>2</sub> )	3d 4d( <sup>3</sup> F <sub>2</sub> )	1778.33	3.35E-01	3.74E-01	5.05E+08		
102	3d 4f( <sup>3</sup> F <sub>2</sub> )	3d 4d( <sup>3</sup> F <sub>2</sub> )	3824.02	1.42E-01	1.12E-01	6.49E+07	2.03E-01	1.70E-01
103	3d 4f( <sup>3</sup> F <sub>2</sub> )	3d 4d( <sup>3</sup> F <sub>3</sub> )	3838.46	1.27E-02	1.00E-02	8.03E+06	1.81E-02	
104	3d 4f( <sup>3</sup> F <sub>3</sub> )	3d 4d( <sup>3</sup> F <sub>3</sub> )	3831.36	1.34E-01	1.06E-01	6.11E+07	1.92E-01	
105	3d 4f( <sup>3</sup> F <sub>4</sub> )	3d 4d( <sup>3</sup> F <sub>3</sub> )	3821.94	1.29E-02	1.01E-02	4.57E+06	1.84E-02	
106	3d 4f( <sup>3</sup> G <sub>3</sub> )	3d 4d( <sup>3</sup> F <sub>3</sub> )	3842.35	3.56E-02	2.83E-02	1.61E+07		
107	3d 4f( <sup>3</sup> G <sub>4</sub> )	3d 4d( <sup>3</sup> F <sub>3</sub> )	3829.07	5.36E-01	4.23E-01	1.90E+08		
108	3d 4f( <sup>3</sup> P <sub>2</sub> )	3d 4d( <sup>3</sup> F <sub>3</sub> )	3799.27	1.37E-02	1.06E-02	8.83E+06		
109	3d 5f( <sup>3</sup> F <sub>3</sub> )	3d 4d( <sup>3</sup> F <sub>3</sub> )	1999.26	1.10E-01	1.70E-01	1.84E+08		
110	3d 5f( <sup>3</sup> F <sub>4</sub> )	3d 4d( <sup>3</sup> F <sub>3</sub> )	1996.68	1.05E-02	1.63E-02	1.37E+07		
111	3d 4f( <sup>3</sup> F <sub>3</sub> )	3d 4d( <sup>3</sup> F <sub>4</sub> )	3850.69	9.95E-03	7.93E-03	5.75E+06	1.42E-02	
112	3d 4f( <sup>3</sup> F <sub>4</sub> )	3d 4d( <sup>3</sup> F <sub>4</sub> )	3841.17	1.50E-01	1.19E-01	6.76E+07		

**Table 3 – continued**

Index	UL.	LL.	$\lambda$	$f_L$	$f_V$	$A_L$	$f$ Ref.[8]	$f_{NIST}$
113	3d 4f ( $^3G_3$ )	3d 4d ( $^3F_4$ )	3861.78	4.38E-04	3.51E-04	2.52E+05		
114	3d 4f ( $^3G_4$ )	3d 4d ( $^3F_4$ )	3848.37	2.77E-02	2.20E-02	1.25E+07		
115	3d 4f ( $^3G_5$ )	3d 4d ( $^3F_4$ )	3831.73	5.44E-01	4.29E-01	2.02E+08		
116	3d 5f ( $^3F_3$ )	3d 4d ( $^3F_4$ )	2004.51	8.16E-03	1.27E-03	1.74E+07		
117	3d 5f ( $^3F_4$ )	3d 4d ( $^3F_4$ )	2001.91	1.23E-01	1.90E-02	2.04E+08		
118	3d 5f ( $^3G_3$ )	3d 4d ( $^3F_4$ )	2001.72	3.60E-04	5.58E-05	7.70E+05		
119	3d 5f ( $^3G_4$ )	3d 4d ( $^3F_4$ )	1998.10	2.27E-02	3.51E-03	3.79E+07		
120	3d 5f ( $^3G_5$ )	3d 4d ( $^3F_4$ )	1993.59	4.45E-01	6.85E-02	6.11E+08		
121	3d 4f ( $^3G_3$ )	3d 4d ( $^3G_4$ )	6708.00	2.95E-13	4.95E-12	5.63E-05		
122	3d 4f ( $^3F_4$ )	3d 4d ( $^3G_4$ )	6646.05	2.57E-14	4.20E-13	3.88E-06		
123	3d 4f ( $^3G_5$ )	3d 4d ( $^3G_4$ )	3378.28	4.86E-03	3.04E-03	2.32E+06		1.0E-01
124	3d 5f ( $^3G_3$ )	3d 4d ( $^3G_4$ )	2566.08	5.44E-13	1.31E-12	7.09E-04		
125	3d 5f ( $^3G_5$ )	3d 4d ( $^3G_4$ )	2552.74	5.50E-13	1.31E-12	4.61E-04		
126	3d 5f ( $^3F_4$ )	3d 4d ( $^3G_4$ )	2566.40	4.67E-14	1.12E-13	4.73E-05		
127	3d 5f ( $^3F_3$ )	3d 4d ( $^3G_4$ )	2570.67	7.00E-13	1.69E-12	9.08E-04		
128	3d 4f( $^1G_4$ )	3d 4d( $^1G_4$ )	3937.69	1.08E-01	7.39E-02	4.63E+07		7.20E-02
129	3d 4f( $^3D_1$ )	3d 4d( $^3P_0$ )	3985.68	5.30E-01	4.13E-01	7.41E+07	7.09E-01	6.30E-01
130	3d 4f( $^3D_1$ )	3d 4d( $^3P_1$ )	3990.90	1.32E-01	1.03E-01	5.54E+07		1.1E-01
131	3d 4f ( $^3P_2$ )	3d 4d ( $^3P_1$ )	3990.94	3.97E-01	3.10E-01	9.97E+07		
132	3d 5p ( $^3F_2$ )	3d 4d ( $^3P_1$ )	7983.88	4.88E-06	4.37E-06	3.07E+01		
133	3d 4f( $^3P_1$ )	3d 4d( $^3P_1$ )	3949.39	6.67E-02	5.11E-02	2.85E+07	9.14E-02	
134	3d 4f( $^3P_2$ )	3d 4d( $^3P_1$ )	3969.76	1.11E-01	8.56E-02	2.81E+07		
135	3d 4f( $^3D_1$ )	3d 4d( $^3P_1$ )	3990.90	1.32E-01	1.03E-01	5.54E+07		
136	3d 4f( $^3P_2$ )	3d 4d( $^3P_2$ )	3982.64	1.93E-01	1.50E-01	8.11E+07		2.5E-01
137	3d 4f ( $^3D_1$ )	3d 4d ( $^3D_1$ )	3311.70	1.78E-01	1.09E-01	1.08E+08	2.44E-01	2.30E-01
138	3d 4f( $^3P_1$ )	3d 4d( $^3D_2$ )	3290.19	1.79E-02	1.09E-02	1.84E+07	2.49E-02	3.1E-02
139	3d 5p( $^1D_2$ )	3d 5s( $^3D_1$ )	7379.45	1.77E-02	2.01E-02	1.30E+06		
140	3d 5p( $^3D_1$ )	3d 5s( $^3D_1$ )	7342.62	1.47E-01	1.66E-01	1.82E+07		
141	3d 5p( $^3F_2$ )	3d 5s( $^3D_2$ )	7286.69	2.66E-02	2.87E-02	3.35E+06		
142	3d 5p( $^3D_2$ )	3d 5s( $^3D_2$ )	7450.25	4.87E-02	5.65E-02	5.85E+06		
143	3d 5p( $^3D_1$ )	3d 5s( $^3D_2$ )	7412.71	2.91E-02	3.35E-02	5.89E+06		
144	3d 5p( $^3D_2$ )	3d 5s( $^3D_2$ )	7365.57	7.54E-02	8.54E-02	9.27E+06		
145	3d 5p( $^3F_3$ )	3d 5s( $^3D_2$ )	7211.62	1.86E-01	2.04E-01	1.70E+07		
146	3d 5p( $^3D_3$ )	3d 5s( $^3D_2$ )	7286.69	1.59E-01	1.77E-01	1.43E+07		
147	3d 5p ( $^3F_2$ )	3d 5s ( $^3D_3$ )	7391.04	5.49E-04	5.72E-04	9.39E+04		
148	3d 5p ( $^3D_2$ )	3d 5s ( $^3D_3$ )	7472.21	1.59E-02	1.85E-02	2.65E+06		
149	3d 5p ( $^3F_3$ )	3d 5s ( $^3D_3$ )	7313.81	1.69E-02	1.77E-02	2.10E+06		
150	3d 5p ( $^3D_3$ )	3d 5s ( $^3D_3$ )	7391.04	8.26E-02	9.43E-02	1.01E+07		
151	3d 5f( $^3G_5$ )	3d 5d( $^3F_4$ )	7972.67	1.21E-01	1.62E-01	1.04E+06		