Fine Structure Calculations of the Energy Levels, Oscillator Strength and Transition Probabilities For as Like Gallium

A.I.Refaie[1], M.S.M.Nour El-Din[2], L.M. Ahamed[2], S.H.Allam[1]
[1]*Physics Dept., Faculty of Science, Benha Univ., Benha, Egypt*
[2]*Physics Dept., Faculty of Science, Cairo Univ., Cairo, Egypt*
E-Mai: mohamed.noureldin@fsc.bu.edu.eg

Abstract

Fine structure calculations of the energy levels, the wavelengths, the oscillator strengths, log gf and the transition probabilities for transitions among the terms belonging to $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$ns, n=5-10, $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$np, n=4-10 , $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$nd, n=4-10 and$1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$nf, n=4-10 configurations of As (III) have been calculated using configurations interaction Cowan atomic structure code. Our calculated values for the above mentioned quantities have been compared with the corresponding experimental data and other theoretical calculations where a satisfactory agreement has been obtained. We also report on some unpublished corresponding values for As like gallium.

Keywords: Energy, Wavelengths, Oscillator srtengths, Transition probabilities .

1. Introduction

Spectroscopic data of gallium [1,2] and gallium-like ions [3-5] may be of interest for plasma investigations in controlled thermonuclear fusion experiments. Recently, multicharged ion spectra of the gallium isoelectronic sequence (Z> 35) have been analyzed. In particular, spectra of the Rb VII ion emitted from sparks and laser-produced plasmas have been investigated [6]. At the same time there are an extensive experimental and theoretical spectroscopic studies for the Gallium like ions. The first six elements of the gallium sequence have been calculated using the multiconfiguration optimised potential model [7].

Gallium isoelectronic sequance has been studied for some transitions using the configuration interaction approach [8]. Multiconfiguration Dirac-Fock calculations on multi-valence-electron systems have been also performed for Ga-like ions [9]. In addition, spectra of the gallium-like ions excited by low-inductance sparks and laser-produced plasmas were observed [10]. Oscillator strengths for excitations of As I-III are calculated using a semiemprical analytic independent-particle-model [11]. Also the energy levels and observed spectral lines of Krypton, Kr I through Kr XXXVI have been studied [12].

The configuration interaction (CI) approach has been used to account for electron correlation effects. To visualize these effects we also include some single configuration results. Two self-consistent-field methods are used to generate orbitals required to construct a multiconfiguration wavefunction. One of them is the Hartree-Fock method with taking into account the relativistic corrections (HFR) and the other one is also Hartree Fock method but without considering the relativistic corrections.

It is found that COWAN code in addition to parametric fit approach is a useful tool for heavy manyelectron systems where intravelence electron correlation plays an essential role. The purpose of this paper is to report new calculations involving higher energy levels, wavelengths, oscillator strengths and transition probabilities that are not calculated before beside the precalculated data to indicate the reliabilities of the new ones by making comparisons with the available theoretical and experimental data.

In the present work, energy levels, wavelengths, log gf, oscillator strengths, and transition probabilities have been calculated for transitions among the terms belonging to to $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$ns, n=5-10, $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$np, n=4-10, $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$nd, n=4-10 and$1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$nf, n=4-10 configurations of As like gallium [13].

2. Method of calculations

Theoretical treatment of an atom containing N electrons requires first of all a knowledge of a suitable Hamiltonian operator. An operator over all N electrons, and adding a term for electrostatic coulomb interactions among electrons [14]

$$H = H_{kin} + H_{elec-nucl} + H_{elec-elec} + H_{S-O} = \sum_{i=1}^{n}\nabla_i^2 - \sum_{i=1}^{N}\frac{2Z}{r_i} + \sum_{i>j}^{N}\sum_{i=1}^{N}\frac{2}{r_{ij}} + \sum_{i=1}^{N}\xi_i(r_i)(l_i - s_i) \quad (1)$$

where $r_i = |r_i|$ is the distance of the ith electron from the nucleus , $r_{ij} = |r_i - r_j|$ is the distance between the ith and j^{th} electron, and $\xi(r_i)$ is a radial proportional factor.It should be noticed that in a multi-electron atom, other magnetic interactions may be considered such as: orbital-orbital, spin-spin, and spin-other orbit interactions. But these interactions are usually much less important than the spin-orbital interaction, thus they can be neglected. Each electron in a many electron atom is considered to move in a central potential independently of the others [15], at least in the first approximation. The ith electron may then be described by the function$\Psi_\alpha(i)$ which is given in terms of a product of radial , spherical harmonic and spin wave functions :-

$$\psi_\alpha(i) = \Psi_{n\ell m_\ell m_s}(i) = R_{n\ell}(r_i)Y_\ell^{m_\ell}(\theta_i,\phi_i)\chi_{m_s}(i) \quad (2)$$

where $R_{n\ell}(r_i)$ is the radial function , $Y_\ell^{m_\ell}(\theta_i,\phi_i)$ is the spherical harmonic function, $\chi_{m_s}(i)$ is the spin function, n is the principal quantum number, m_ℓ is the z-component of the electron orbital angular momentum quantum number, and m_s is the z-component of the electron spin quantum number.

For N-electrons, the Pauli principle requires that each set of quantum numbers: α, β, γ, ……..ν should be different from one electron to other . This means that a simple N-electron wave function will consist of a direct product of single-electron wave functions:

$$\psi_\alpha(1)\psi_\beta(2)\psi_\gamma(3)..........................\psi_\nu(N)$$ The Pauli principle can be included in a more general symmetry principle, produced by Heisenberg and Dirac. Slater showed that this requirement could be satisfied by a normalized determinatal product wave function of the form:-

$$\psi(\alpha,\beta,........\nu) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_\alpha(1) & \psi_\alpha(2) & .... & \psi_\alpha(N) \\ \psi_\beta(1) & \psi_\beta(2) & & \psi_\beta(N) \\ .... & & & \\ \psi_\nu(1) & \psi_\nu(2) & .... & \psi_\nu(N) \end{vmatrix} \quad (3)$$

In practice the linear combinations of such determinant functions for single configurations are formed which are angular eigenstates in an appropriate coupling scheme and these form the basis states for the multi-configuration expansions.

The matrix elements of the Hamiltonian between determinant functions can be reduced to one and two electron terms so that for states B and B′ [13]:

$$\langle B|H|B'\rangle = E_{av}\delta_{BB'} + \sum_{ijk}[f_k F^k(\ell_i\ell_j) + g_k G^k(\ell_i\ell_j)] + \sum_i d_i\zeta(\ell_i) \quad (4)$$

where E_{av} is the central field energy. Furthermore, modest ad hoc scaling adjustments are applied to the F, G, and d to allow for configurations omitted from the multi-configuration expansion. The wave functions obtained from equation (3) are used to calculate the excitation energies of the fine structure levels, the oscillator strengths and the transition probabilities. The calculations are carried out in intermediate coupling scheme. A choice of nomenclatures is possible in seeking to assign angular quantum numbers as identifiers of the intermediate coupling numerical eigen states. Since only parity and total angular momentum observables commute with the Hamiltonian, other quantum number assignments are approximated one. In these assignments we are led by angular momentum coupling schemes appropriate to the dominant parts of the Hamiltonian. One of them is known as the LS-scheme when the electrostatic terms dominate and the other is known as the jj-scheme when relativistic terms dominate. The code identifies the energy eigen states by dominant component in its expansion in a particular basis.

The radial function is obtained as the solution of the following equation [13,16]:

$$\left[\frac{d^2}{dr^2} + \frac{\ell_i(\ell_i+1)}{r^2} + V_i(r)\right]_i R_{nl}(r) = \varepsilon_i R_{nl}(r)$$

The solution of the above Shrodinger equation (the radial wave function R_{nl}®) is analogous to the behavior of legender P_{nl}® for which we have

$$\int_0^\infty P_{n\ell}(r)\,P_{n'\ell}(r)\,dr = \delta_{nn'} \quad ; \quad \ell+1 < n' \le n$$

where V_i is the central potential seen by the ith electron and ε_i is the single particle energy. An optimised potential is obtained variationally. It is noticeable that the present code uses the Relativistic Hartree Fock method of Cowan [13].

2.1 Spontaneous transitions between degenerate levels

The radiative decay rate between degenerate levels p and q is given by [17]:

$$A_{pq} = \frac{e^2 w_{pq}^3}{3\pi\varepsilon_o \hbar c^3}\sum_{m_q}\left|<qm_q|r|pm_p>\right|^2 \quad (5)$$

where m_p and m_q are the magnetic orbital quantum numbers of the involved levels, e is the electron charge, c is the speed of light, W is the angular frequency of the transition photon, and ε_o is the vacuum permittivity.

The decay rate can be made more symmetrical by introducing an additional summation over mp and dividing by the statistical weight $g_p = 2j_p + 1$ of the upper level:

$$A_{pq} = \frac{e^2 w_{pq}^3}{3\pi\varepsilon_o \hbar c^3}\frac{1}{g_p}\sum_{m_p m_q}\left|<qm_q|r|pm_p>\right|^2 \quad (6)$$

The radiative life time τ_p of an excited atomic state p is related to the atomic transition probability Apq by:

$$\tau_p = 1/\sum A_{pq} \quad (7)$$

where, the sum is extended over all the lower states which can be reached from the upper state by radiative decay.

2.2 Oscillator strengths

The oscillator strength or f-value describes what fraction of the energy of the classical oscillator should be ascribed to a given transition [17]. For transitions from an upper level p to a lower level q, the emission f-value, f_{pq} is given by the following relation.

$$A_{pq} = -3f_{pq}\gamma \quad (8)$$

where:

$$\gamma = \frac{e^2 w^3}{6\pi\varepsilon_o mc^3}$$

is defined as the classical transition probability. While for an upward transition from level q to level p, the absorption f-value, f_{qp}, is defined by:

$$g_q f_{qp} = -g_p f_{pq} \quad (9)$$

The explicit expressions for the transition probability A_{pq} in terms of the emission and the

absorption oscillator strengths are given now by the following relation:

$$A_{pq} = \frac{e^2 w_{pq}^3}{2\pi\varepsilon_o mc^3}(-f_{pq}) = \frac{e^2 w_{qp}^3}{2\pi\varepsilon_o mc^3}(\frac{g_q}{g_p}f_{qp}) \qquad (10)$$

3. Results and discussion
3.1 Energy levels

In general, with one electron outside a closed shell, correlation in the core is negligible [14]. The energy of the electronic configurations are obtained by adjusting the scalling parameters E_{av} and ζ_i (r_i) that are shown in Table (1)The energy levels for As like gallium have been tabulated in Table (2) Our

calculations of energy levels have been compared with data relative to NIST From the comparison we found that all the calculated energy levels are almost the same to the valuse of NIST [18].

3.2 Wavelengths, oscillator strengths and transition probabilities

In Table (3) we have tabulated our calculated wavelengths, λ (Å), the absorption oscillator strength, f, log(Gf) and the radiative decay rates, A, for all allowed electric dipole transitions among As III [19].

Table (1) Radial function parameters for for Gallium-like ions in units of 1000 cm⁻¹.

Configuration	Parameter	Ion
		As III
$4s^24p$	E_{av}	1.9600
	ζ_i (r_i)	1.9600
$4s^25p$	E_{av}	131.9407
	ζ_i (r_i)	0.4827
$4s^26p$	E_{av}	174.2346
	ζ_i (r_i)	0.1856
$4s^27p$	E_{av}	193.3800
	ζ_i (r_i)	0.0975
$4s^28p$	E_{av}	203.9731
	ζ_i (r_i)	0.0576
$4s^29p$	E_{av}	210.4644
	ζ_i (r_i)	0.0369
$4s^210p$	E_{av}	214.7338
	ζ_i (r_i)	0.0250
$4s^24f$	E_{av}	164.1104
	ζ_i (r_i)	-0.0100
$4s^25f$	E_{av}	188.4820
	ζ_i (r_i)	0.0003
$4s^26f$	E_{av}	201.0537
	ζ_i (r_i)	0.0002
$4s^27f$	E_{av}	208.5886
	ζ_i (r_i)	0.0001
$4s^28f$	E_{av}	213.4606
	ζ_i (r_i)	0.0001
$4s^29f$	E_{av}	216.7884
	ζ_i (r_i)	0.0000
$4s^210f$	E_{av}	219.1616
	ζ_i (r_i)	0.0000
$4s^25s$	E_{av}	106.6940
$4s^26s$	E_{av}	162.8890
$4s^27s$	E_{av}	184.1295
$4s^28s$	E_{av}	200.8780
$4s^29s$	E_{av}	208.5050
$4s^210s$	E_{av}	213.4160
$4s^24d$	E_{av}	117.7068
	ζ_i (r_i)	0.0372
$4s^25d$	E_{av}	165.6740
	ζ_i (r_i)	0.0340
$4s^26d$	E_{av}	189.2677
	ζ_i (r_i)	0.0130
$4s^27d$	E_{av}	201.5790
	ζ_i (r_i)	0.0075
$4s^28d$	E_{av}	208.9466
	ζ_i (r_i)	0.0047
$4s^29d$	E_{av}	213.7121
	ζ_i (r_i)	0.0031
$4s^210d$	E_{av}	216.9712
	ζ_i (r_i)	0.0022

Table (2) Energy levels in cm^{-1} for As III calculated by COWAN code in Comparison with NIST experimental values

Levels	Energy	NIST	Dev. % Relative to NIST
$4s^24p(^2P_{1/2})$	0.00	0.00	0
$4s^24p(^2P_{3/2})$	2940.00	2940.00	0
$4s^25s(^2S_{1/2})$	106694.00	106694.00	0
$4s^24d(^2D_{3/2})$	117651.00	117651.00	0
$4s^24d(^2D_{5/2})$	117744.00	117744.00	0
$4s^25p(^2P_{1/2})$	131458.00	131458.00	0
$4s^25p(^2P_{3/2})$	132182.10	132182.00	-7.57E-05
$4s^26s(^2S_{1/2})$	162889.50	162889.50	0
$4s^24f(^2F_{7/2})$	164095.40	164107.00	7.07E-03
$4s^24f(^2F_{5/2})$	164130.40	164115.00	-9.38E-03
$4s^25d(^2D_{3/2})$	165623.00	165623.00	0
$4s^25d(^2D_{5/2})$	165708.00	165708.00	0
$4s^26p(^2P_{1/2})$	174049.00	---	---
$4s^26p(^2P_{3/2})$	174327.40	---	---
$4s^27s(^2S_{1/2})$	184129.50	---	---
$4s^25f(^2F_{5/2})$	188481.40	---	---
$4s^25f(^2F_{7/2})$	188482.50	---	---
$4s^26d(^2D_{3/2})$	189248.20	---	---
$4s^26d(^2D_{5/2})$	189280.70	---	---
$4s^27p(^2P_{1/2})$	193282.50	---	---
$4s^27p(^2P_{3/2})$	193428.80	---	---
$4s^28s(^2S_{1/2})$	200878.90	---	---
$4s^26f(^2F_{5/2})$	201053.30	---	---
$4s^26f(^2F_{7/2})$	201054.00	---	---
$4s^27d(^2D_{3/2})$	201567.80	---	---
$4s^27d(^2D_{5/2})$	201586.50	---	---
$4s^28p(^2P_{1/2})$	203915.50	---	---
$4s^28p(^2P_{3/2})$	204001.90	---	---
$4s^29s(^2S_{1/2})$	208505.20	---	---
$4s^27f(^2F_{5/2})$	208588.40	---	---
$4s^27f(^2F_{7/2})$	208588.80	---	---
$4s^28d(^2D_{3/2})$	208939.50	---	---
$4s^28d(^2D_{5/2})$	208951.30	---	---
$4s^29p(^2P_{1/2})$	210427.50	---	---
$4s^29p(^2P_{3/2})$	210482.90	---	---
$4s^210s(^2S_{1/2})$	213416.60	---	---
$4s^28f(^2F_{5/2})$	213460.40	---	---
$4s^28f(^2F_{7/2})$	213460.70	---	---
$4s^29d(^2D_{3/2})$	213707.40	---	---
$4s^29d(^2D_{5/2})$	213715.20	---	---
$4s^210p(^2P_{1/2})$	214708.80	---	---
$4s^210p(^2P_{3/2})$	214746.30	---	---
$4s^29f(^2F_{5/2})$	216788.40	---	---
$4s^29f(^2F_{7/2})$	216788.40	---	---
$4s^210d(^2D_{3/2})$	216967.90	---	---
$4s^210d(^2D_{5/2})$	216973.40	---	---
$4s^210f(^2F_{5/2})$	219161.60	---	---
$4s^210f(^2F_{7/2})$	219161.60	---	---

Table (3) Wavelengths, log gf, oscillator strengths and radiative decay rates for As III.

λ (Å)	upper levels	lower levels	Log(G f)	f	A(s^{-1})
460.90	$4s^2 10d(^2D_{3/2})$	$4s^2 4p(^2P_{1/2})$	-2.330	2.34E-03	3.68E+07
467.22	$4s^2 10d(^2D_{5/2})$	$4s^2 4p(^2P_{3/2})$	-2.081	2.07E-03	4.23E+07
467.23	$4s^2 10d(^2D_{3/2})$	$4s^2 4p(^2P_{3/2})$	-3.035	2.30E-04	7.05E+06
467.93	$4s^2 9d(^2D_{3/2})$	$4s^2 4p(^2P_{1/2})$	-2.145	3.58E-03	5.45E+07
468.57	$4s^2 10s(^2S_{1/2})$	$4s^2 4p(^2P_{1/2})$	-2.494	1.60E-03	4.87E+07
474.44	$4s^2 9d(^2D_{5/2})$	$4s^2 4p(^2P_{3/2})$	-1.896	3.17E-03	6.28E+07
474.46	$4s^2 9d(^2D_{3/2})$	$4s^2 4p(^2P_{3/2})$	-2.850	3.53E-04	1.05E+07
475.11	$4s^2 10s(^2S_{1/2})$	$4s^2 4p(^2P_{3/2})$	-2.199	1.58E-03	9.35E+07
478.61	$4s^2 8d(^2D_{3/2})$	$4s^2 4p(^2P_{1/2})$	-1.925	5.94E-03	8.65E+07
479.60	$4s^2 9s(^2S_{1/2})$	$4s^2 4p(^2P_{1/2})$	-2.296	2.53E-03	7.35E+07
485.41	$4s^2 8d(^2D_{5/2})$	$4s^2 4p(^2P_{3/2})$	-1.676	5.27E-03	9.95E+07
485.44	$4s^2 8d(^2D_{3/2})$	$4s^2 4p(^2P_{3/2})$	-2.630	5.85E-04	1.66E+07
486.46	$4s^2 9s(^2S_{1/2})$	$4s^2 4p(^2P_{3/2})$	-2.002	2.49E-03	1.41E+08
496.11	$4s^2 7d(^2D_{3/2})$	$4s^2 4p(^2P_{1/2})$	-1.652	1.11E-02	1.51E+08
497.81	$4s^2 8s(^2S_{1/2})$	$4s^2 4p(^2P_{1/2})$	-2.057	4.38E-03	1.18E+08
503.41	$4s^2 7d(^2D_{5/2})$	$4s^2 4p(^2P_{3/2})$	-1.403	9.88E-03	1.73E+08
503.45	$4s^2 7d(^2D_{3/2})$	$4s^2 4p(^2P_{3/2})$	-2.358	1.10E-03	2.90E+07
505.21	$4s^2 8s(^2S_{1/2})$	$4s^2 4p(^2P_{3/2})$	-1.763	4.31E-03	2.26E+08
528.41	$4s^2 6d(^2D_{3/2})$	$4s^2 4p(^2P_{1/2})$	-1.289	2.57E-02	3.08E+08
536.65	$4s^2 6d(^2D_{5/2})$	$4s^2 4p(^2P_{3/2})$	-1.040	2.28E-02	3.52E+08
536.75	$4s^2 6d(^2D_{3/2})$	$4s^2 4p(^2P_{3/2})$	-1.994	2.53E-03	5.88E+07
543.10	$4s^2 7s(^2S_{1/2})$	$4s^2 4p(^2P_{1/2})$	-1.762	8.64E-03	1.96E+08
551.91	$4s^2 7s(^2S_{1/2})$	$4s^2 4p(^2P_{3/2})$	-1.468	8.51E-03	3.73E+08
603.78	$4s^2 5d(^2D_{3/2})$	$4s^2 4p(^2P_{1/2})$	-0.747	8.95E-02	8.20E+08
613.91	$4s^2 6s(^2S_{1/2})$	$4s^2 4p(^2P_{1/2})$	-1.325	2.36E-02	4.19E+08
614.37	$4s^2 5d(^2D_{5/2})$	$4s^2 4p(^2P_{3/2})$	-0.499	7.92E-02	9.33E+08
614.69	$4s^2 5d(^2D_{3/2})$	$4s^2 4p(^2P_{3/2})$	-1.453	8.80E-03	1.55E+08
625.20	$4s^2 6s(^2S_{1/2})$	$4s^2 4p(^2P_{3/2})$	-1.031	2.33E-02	7.95E+08
849.97	$4s^2 4d(^2D_{3/2})$	$4s^2 4p(^2P_{1/2})$	0.354	1.13E+00	5.23E+09
871.05	$4s^2 4d(^2D_{5/2})$	$4s^2 4p(^2P_{3/2})$	0.599	9.93E-01	5.82E+09
871.76	$4s^2 4d(^2D_{3/2})$	$4s^2 4p(^2P_{3/2})$	-0.356	1.10E-01	9.68E+08
925.48	$4s^2 10p(^2P_{3/2})$	$4s^2 5s(^2S_{1/2})$	-3.699	9.98E-05	3.90E+05
925.80	$4s^2 10p(^2P_{1/2})$	$4s^2 5s(^2S_{1/2})$	-4.000	4.99E-05	3.89E+05
937.26	$4s^2 5s(^2S_{1/2})$	$4s^2 4p(^2P_{1/2})$	-0.524	1.50E-01	1.14E+09
963.50	$4s^2 9p(^2P_{3/2})$	$4s^2 5s(^2S_{1/2})$	-3.596	1.27E-04	4.55E+05
963.82	$4s^2 5s(^2S_{1/2})$	$4s^2 4p(^2P_{3/2})$	-0.235	1.46E-01	2.09E+09
964.01	$4s^2 9p(^2P_{1/2})$	$4s^2 5s(^2S_{1/2})$	-3.897	6.33E-05	4.55E+05
985.12	$4s^2 10f(^2F_{5/2})$	$4s^2 4d(^2D_{3/2})$	-1.713	4.84E-03	2.22E+07
986.02	$4s^2 10f(^2F_{5/2})$	$4s^2 4d(^2D_{5/2})$	-2.859	2.30E-04	1.58E+06
986.02	$4s^2 10f(^2F_{7/2})$	$4s^2 4d(^2D_{5/2})$	-1.558	4.61E-03	2.38E+07
1008.70	$4s^2 9f(^2F_{5/2})$	$4s^2 4d(^2D_{3/2})$	-1.536	7.27E-03	3.18E+07
1009.65	$4s^2 9f(^2F_{5/2})$	$4s^2 4d(^2D_{5/2})$	-2.682	3.46E-04	2.27E+06
1009.65	$4s^2 9f(^2F_{7/2})$	$4s^2 4d(^2D_{5/2})$	-1.381	6.93E-03	3.40E+07
1027.67	$4s^2 8p(^2P_{3/2})$	$4s^2 5s(^2S_{1/2})$	-3.541	1.44E-04	4.55E+05
1028.58	$4s^2 8p(^2P_{1/2})$	$4s^2 5s(^2S_{1/2})$	-3.842	7.18E-05	4.53E+05
1029.92	$4s^2 10p(^2P_{3/2})$	$4s^2 4d(^2D_{3/2})$	-3.733	4.62E-05	2.90E+05
1030.31	$4s^2 10p(^2P_{1/2})$	$4s^2 4d(^2D_{3/2})$	-3.035	2.30E-04	2.90E+06
1030.90	$4s^2 10p(^2P_{3/2})$	$4s^2 4d(^2D_{5/2})$	-2.780	2.76E-04	2.60E+06
1043.74	$4s^2 8f(^2F_{5/2})$	$4s^2 4d(^2D_{3/2})$	-1.326	1.18E-02	4.82E+07
1044.75	$4s^2 8f(^2F_{7/2})$	$4s^2 4d(^2D_{5/2})$	-1.171	1.12E-02	5.15E+07
1044.75	$4s^2 8f(^2F_{5/2})$	$4s^2 4d(^2D_{5/2})$	-2.472	5.62E-04	3.43E+06

Table (3) Continue

1077.22	$4s^29p(^2P_{3/2})$	$4s^24d(^2D_{3/2})$	-3.536	7.27E-05	4.18E+05
1077.86	$4s^29p(^2P_{1/2})$	$4s^24d(^2D_{3/2})$	-2.837	3.63E-04	4.18E+06
1078.30	$4s^29p(^2P_{3/2})$	$4s^24d(^2D_{5/2})$	-2.582	4.36E-04	3.75E+06
1099.66	$4s^27f(^2F_{5/2})$	$4s^24d(^2D_{3/2})$	-1.067	2.14E-02	7.87E+07
1100.78	$4s^27f(^2F_{7/2})$	$4s^24d(^2D_{5/2})$	-0.913	2.04E-02	8.41E+07
1100.78	$4s^27f(^2F_{5/2})$	$4s^24d(^2D_{5/2})$	-2.214	1.02E-03	5.60E+06
1152.94	$4s^27p(^2P_{3/2})$	$4s^25s(^2S_{1/2})$	-3.783	8.23E-05	2.07E+05
1154.89	$4s^27p(^2P_{1/2})$	$4s^25s(^2S_{1/2})$	-4.085	4.10E-05	2.06E+05
1158.07	$4s^28p(^2P_{3/2})$	$4s^24d(^2D_{3/2})$	-3.295	1.27E-04	6.30E+05
1159.23	$4s^28p(^2P_{1/2})$	$4s^24d(^2D_{3/2})$	-2.596	6.33E-04	6.30E+06
1159.31	$4s^28p(^2P_{3/2})$	$4s^24d(^2D_{5/2})$	-2.341	7.59E-04	5.65E+06
1169.46	$4s^210d(^2D_{3/2})$	$4s^25p(^2P_{1/2})$	-1.951	5.59E-03	1.36E+07
1179.37	$4s^210d(^2D_{5/2})$	$4s^25p(^2P_{3/2})$	-1.700	4.98E-03	1.60E+07
1179.44	$4s^210d(^2D_{3/2})$	$4s^25p(^2P_{3/2})$	-2.654	5.54E-04	2.65E+06
1199.01	$4s^26f(^2F_{5/2})$	$4s^24d(^2D_{3/2})$	-0.732	4.63E-02	1.44E+08
1200.34	$4s^26f(^2F_{7/2})$	$4s^24d(^2D_{5/2})$	-0.577	4.41E-02	1.54E+08
1200.35	$4s^26f(^2F_{5/2})$	$4s^24d(^2D_{5/2})$	-1.878	2.21E-03	1.02E+07
1215.81	$4s^29d(^2D_{3/2})$	$4s^25p(^2P_{1/2})$	-1.739	9.11E-03	2.06E+07
1220.13	$4s^210s(^2S_{1/2})$	$4s^25p(^2P_{1/2})$	-2.172	3.36E-03	1.51E+07
1226.50	$4s^29d(^2D_{5/2})$	$4s^25p(^2P_{3/2})$	-1.488	8.12E-03	2.40E+07
1226.61	$4s^29d(^2D_{3/2})$	$4s^25p(^2P_{3/2})$	-2.442	9.03E-04	4.00E+06
1231.00	$4s^210s(^2S_{1/2})$	$4s^25p(^2P_{3/2})$	-1.875	3.33E-03	2.94E+07
1290.63	$4s^28d(^2D_{3/2})$	$4s^25p(^2P_{1/2})$	-1.476	1.67E-02	3.35E+07
1297.91	$4s^29s(^2S_{1/2})$	$4s^25p(^2P_{1/2})$	-1.934	5.82E-03	2.31E+07
1302.61	$4s^28d(^2D_{5/2})$	$4s^25p(^2P_{3/2})$	-1.224	1.49E-02	3.92E+07
1302.80	$4s^28d(^2D_{3/2})$	$4s^25p(^2P_{3/2})$	-2.179	1.65E-03	6.53E+06
1310.22	$4s^29s(^2S_{1/2})$	$4s^25p(^2P_{3/2})$	-1.637	5.76E-03	4.48E+07
1319.65	$4s^27p(^2P_{3/2})$	$4s^24d(^2D_{3/2})$	-2.979	2.62E-04	1.01E+06
1321.27	$4s^27p(^2P_{3/2})$	$4s^24d(^2D_{5/2})$	-2.025	1.57E-03	9.03E+06
1322.20	$4s^27p(^2P_{1/2})$	$4s^24d(^2D_{3/2})$	-2.281	1.31E-03	1.00E+07
1411.82	$4s^25f(^2F_{5/2})$	$4s^24d(^2D_{3/2})$	-0.253	1.40E-01	3.12E+08
1413.66	$4s^25f(^2F_{7/2})$	$4s^24d(^2D_{5/2})$	-0.098	1.33E-01	3.33E+08
1413.68	$4s^25f(^2F_{5/2})$	$4s^24d(^2D_{5/2})$	-1.400	6.63E-03	2.22E+07
1426.34	$4s^27d(^2D_{3/2})$	$4s^25p(^2P_{1/2})$	-1.126	3.74E-02	6.13E+07
1440.49	$4s^28s(^2S_{1/2})$	$4s^25p(^2P_{1/2})$	-1.625	1.18E-02	3.81E+07
1440.83	$4s^27d(^2D_{5/2})$	$4s^25p(^2P_{3/2})$	-0.876	3.32E-02	7.13E+07
1441.22	$4s^27d(^2D_{3/2})$	$4s^25p(^2P_{3/2})$	-1.830	3.69E-03	1.19E+07
1455.67	$4s^28s(^2S_{1/2})$	$4s^25p(^2P_{3/2})$	-1.329	1.17E-02	7.40E+07
1478.56	$4s^26p(^2P_{3/2})$	$4s^25s(^2S_{1/2})$	-3.048	4.47E-04	6.83E+05
1484.67	$4s^26p(^2P_{1/2})$	$4s^25s(^2S_{1/2})$	-3.350	2.23E-04	6.75E+05
1730.40	$4s^26d(^2D_{3/2})$	$4s^25p(^2P_{1/2})$	-0.609	1.23E-01	1.37E+08
1751.36	$4s^26d(^2D_{5/2})$	$4s^25p(^2P_{3/2})$	-0.359	1.09E-01	1.59E+08
1752.35	$4s^26d(^2D_{3/2})$	$4s^25p(^2P_{3/2})$	-1.313	1.22E-02	2.65E+07
1764.40	$4s^26p(^2P_{3/2})$	$4s^24d(^2D_{3/2})$	-2.493	8.03E-04	1.72E+06
1767.30	$4s^26p(^2P_{3/2})$	$4s^24d(^2D_{5/2})$	-1.539	4.81E-03	1.54E+07
1773.11	$4s^26p(^2P_{1/2})$	$4s^24d(^2D_{3/2})$	-1.796	4.00E-03	1.70E+07
1867.81	$4s^210f(^2F_{5/2})$	$4s^25d(^2D_{3/2})$	-1.311	1.22E-02	1.56E+07
1870.78	$4s^210f(^2F_{5/2})$	$4s^25d(^2D_{5/2})$	-2.458	5.80E-04	1.11E+06
1870.78	$4s^210f(^2F_{7/2})$	$4s^25d(^2D_{5/2})$	-1.157	1.16E-02	1.66E+07
1891.15	$4s^210d(^2D_{5/2})$	$4s^24f(^2F_{7/2})$	-3.420	4.75E-05	1.18E+05
1892.60	$4s^210d(^2D_{3/2})$	$4s^24f(^2F_{5/2})$	-3.575	4.43E-05	1.24E+05
1898.56	$4s^27s(^2S_{1/2})$	$4s^25p(^2P_{1/2})$	-1.206	3.11E-02	5.75E+07
1925.02	$4s^27s(^2S_{1/2})$	$4s^25p(^2P_{3/2})$	-0.911	3.07E-02	1.11E+08
1928.39	$4s^210p(^2P_{3/2})$	$4s^26s(^2S_{1/2})$	-3.802	7.88E-05	7.08E+04
1929.78	$4s^210p(^2P_{1/2})$	$4s^26s(^2S_{1/2})$	-4.104	3.93E-05	7.05E+04
1954.45	$4s^29f(^2F_{5/2})$	$4s^25d(^2D_{3/2})$	-1.113	1.93E-02	2.25E+07
1957.70	$4s^29f(^2F_{5/2})$	$4s^25d(^2D_{5/2})$	-2.260	9.15E-04	1.60E+06
1957.70	$4s^29f(^2F_{7/2})$	$4s^25d(^2D_{5/2})$	-0.959	1.83E-02	2.39E+07
2015.33	$4s^29d(^2D_{5/2})$	$4s^24f(^2F_{7/2})$	-3.155	8.74E-05	1.92E+05

Table (3) Continue

2017.06	$4s^29d(^2D_{3/2})$	$4s^24f(^2F_{5/2})$	-3.310	8.15E-05	2.01E+05
2035.69	$4s^210p(^2P_{3/2})$	$4s^25d(^2D_{3/2})$	-3.530	7.37E-05	1.19E+05
2037.25	$4s^210p(^2P_{1/2})$	$4s^25d(^2D_{3/2})$	-2.831	3.68E-04	1.19E+06
2039.22	$4s^210p(^2P_{3/2})$	$4s^25d(^2D_{5/2})$	-2.576	4.42E-04	1.06E+06
2090.42	$4s^28f(^2F_{5/2})$	$4s^25d(^2D_{3/2})$	-0.871	3.36E-02	3.42E+07
2094.12	$4s^28f(^2F_{7/2})$	$4s^25d(^2D_{5/2})$	-0.717	3.20E-02	3.65E+07
2094.14	$4s^28f(^2F_{5/2})$	$4s^25d(^2D_{5/2})$	-2.018	1.60E-03	2.43E+06
2101.13	$4s^29p(^2P_{3/2})$	$4s^26s(^2S_{1/2})$	-3.901	6.27E-05	4.75E+04
2152.42	$4s^24f(^2F_{5/2})$	$4s^24d(^2D_{3/2})$	0.572	9.33E-01	8.97E+08
2155.80	$4s^24f(^2F_{5/2})$	$4s^24d(^2D_{5/2})$	-0.575	4.43E-02	6.37E+07
2157.43	$4s^24f(^2F_{7/2})$	$4s^24d(^2D_{5/2})$	0.726	8.87E-01	9.53E+08
2229.17	$4s^29p(^2P_{3/2})$	$4s^25d(^2D_{3/2})$	-3.292	1.27E-04	1.72E+05
2229.36	$4s^28d(^2D_{5/2})$	$4s^24f(^2F_{7/2})$	-2.809	1.94E-04	3.47E+05
2231.10	$4s^28d(^2D_{5/2})$	$4s^24f(^2F_{5/2})$	-4.111	1.29E-05	1.73E+04
2231.69	$4s^28d(^2D_{3/2})$	$4s^24f(^2F_{5/2})$	-2.965	1.80E-04	3.63E+05
2231.92	$4s^29p(^2P_{1/2})$	$4s^25d(^2D_{3/2})$	-2.593	6.37E-04	1.71E+06
2233.40	$4s^29p(^2P_{3/2})$	$4s^25d(^2D_{5/2})$	-2.338	7.65E-04	1.54E+06
2327.45	$4s^27f(^2F_{5/2})$	$4s^25d(^2D_{3/2})$	-0.561	6.87E-02	5.65E+07
2329.98	$4s^210d(^2D_{3/2})$	$4s^26p(^2P_{1/2})$	-1.604	1.24E-02	7.65E+06
2332.05	$4s^27f(^2F_{7/2})$	$4s^25d(^2D_{5/2})$	-0.407	6.53E-02	6.01E+07
2332.07	$4s^27f(^2F_{5/2})$	$4s^25d(^2D_{5/2})$	-1.708	3.26E-03	4.00E+06
2344.89	$4s^210d(^2D_{5/2})$	$4s^26p(^2P_{3/2})$	-1.351	1.11E-02	9.00E+06
2345.19	$4s^210d(^2D_{3/2})$	$4s^26p(^2P_{3/2})$	-2.306	1.23E-03	1.50E+06
2521.53	$4s^29d(^2D_{3/2})$	$4s^26p(^2P_{1/2})$	-1.349	2.24E-02	1.18E+07
2538.86	$4s^29d(^2D_{5/2})$	$4s^26p(^2P_{3/2})$	-1.096	2.00E-02	1.38E+07
2539.36	$4s^29d(^2D_{3/2})$	$4s^26p(^2P_{3/2})$	-2.051	2.22E-03	2.30E+06
2540.16	$4s^210s(^2S_{1/2})$	$4s^26p(^2P_{1/2})$	-1.820	7.56E-03	7.80E+06

4. Conclusion

It is clear that the present calculations of energy levels and wavelengths show good agreement with the corresponding available both theoretical and experimental data. We have obtained some new unpublished energy levels, wavelengths and transition probabilities for these ions. These extensive and the more definitive results may be useful in thermonuclear fusion research and astrophysical applications.

References

[1] D.Iablonskyi, K..Jänkälä, S.Urpelainen and M.Huttula, J.Phys. B: At. Mol. Opt.Phys.46, 175001 , 2013.

[2] Yu.M.Smirnov, Opt. Spectrosc.110, pp.1–8, 2011.

[3] J.E.Sansonetti, J.Phys. Chem. Ref. Data 41, 01310 , 2012.

[4] J.E.Sansonetti, J.Phys. Chem. Ref. Data 35, 301, 2006.

[5] J.E.Sansonetti and W.C.Martin, J.Phys.Chem. Ref. Data 34, 1559, 2005.

[6]E.Biémont, P.Quinet, J.Quant. spectrosc. Radiat. Transfer Vol.44, (2), pp.233- 244, 1990.

[7] K.Aashamar, T.M.Luke and J.D.Talman, J.Phys. B: At. Mol. Phys. 16, pp.2695-2708, 1983.

[8] R.Marcinek and J.Migdalek, J.Phys. B: At. Mol. Opt. Phys. 26, PP.1403-1414, 1993.

[9] F.Hu, J.Yag, C.Wang, L.Jing, S.Chen, G.Jiang, H.Liu, L.Hao; Phys. Rev. A 84, 04250 , 2011.

[10] J.Reader, N.Acquista, and S.Goldsmith, J. Opt. Soc. Am. B, vol.3, p.874, 1986.

[11] P.S.Ganas, Astron. Astrophys., Suppl.Ser. pp.143, 491, 2000.

[12] E.B.Saloman, J.Phys. Chem. Ref. Data 36, p.215, 2007.

[13] http://www.tcd.ie/Physics/People/Cormac.McGuinness/Cowan/.

[14] R.D.Cowan, The theory of atomic structure and spectra, University of California Press, Berkeley-Los Angeles-London, 1981.

[15] Sobelman "Introduction to the Theory of Atomic Spectra", international series of monographs in Natural Philosophy ,Pergamon Press,Vol.40, 1979.

[16] J.C.Slater, "Quantum Theory of Atomic Structure", Vols.I and II, McGraw-Hill, New York, 1960.

[17] Alan Corney "Atomic And Laser Spectroscopy"Oxford Univesity Press, 1977.

[18] D.E.Kellcher, W.C.Martin., W.L.Wiese, J.Suger, J.RFuher, K.Olsen, A.Musgrove, P. J. Mohr, J. Reader and G. R. Dalton, Phys. Scr. Vol.83, p.158, 1999. http://physics.nist.gov/cgi-bin/atdata/main_asd.

[19] A.Hibbert, in:W.Hanle, H.Kleinpoppen (Eds.), Atomic Structure Theory in Progress in Atomic Spectroscopy, Plenum, New York, , p.1, 1979.