

# Configuration Interaction Calculations of Energy Levels and Radiative Parameters of Calcium-Like Ions, $22 \leq Z \leq 30$

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**Abstract:** The energy levels, oscillator strengths, and E1 transition probabilities have been calculated for calcium-like ions with  $Z = 22 - 30$  (excluding iron). The calculations have been executed using the CIV3 and LANL codes for a set of configuration arrays including 63 fine structure levels (in this paper we mentioned for examples about 40 energy levels) belonging to  $3p^6 3d^2$  and  $3p^6 3d4l$  configurations, where  $l = s, p, d, f$ . The correlations up to  $6l$  orbitals are included to optimize the wave functions generated by the CIV3 code. In spite of the complexity of the Ca sequence, the present results are in fairly good agreement with the experimental and theoretical data available in the literature. The present study provides calculations of various atomic structure data which are necessary for many fields of researches and applications, especially in the astrophysics and plasma diagnostics.

**Keywords:** Energy Level, Oscillator Strength, Radiative Rates, Configuration Interaction

## 1. Introduction

Members of the calcium isoelectronic sequence such as vanadium, iron, cobalt, and nickel are of importance for astrophysics as well as for plasma modeling. The importance of calcium-like ions (vanadium through zinc) for astrophysics lies within its abundance in the solar system, so, transitions arise from these atomic systems possible to appear in the solar spectra and in stellar corona. The spectra of calcium isoelectronic sequence had been studied early by many authors [1–4], these works had provided results of observed transition parameters and energies of Ca-like manganese, scandium, cobalt, iron, nickel, copper, and zinc. Fawcett and Cowan [5] have studied the spectral lines arise from Ca-like iron (Fe VII), the atomic self-consistent field calculations have been applied to identify the spectra belonging to the  $3d^2 - 3p^5 3d^3$  transition arrays. The spectrum of Fe VII has been observed by Ekberg [6] using low- and high-voltage sliding spark, as well as the Fe VII spectra has

been studied in many other different works such as [7–20]. A measured values of lifetimes for some transitions of the  $3d^2 \rightarrow 3d4p$  arrays in Ti III have been reported [21, 22] using the beam-foil technique. Abbott [23] has used the non-relativistic SUPERSTRUCTURE program to calculate the transition probabilities of calcium-like ionized Cr, Mn, Fe, and Ni, the calculations have been carried out for transitions belonging to  $3d^2$ ,  $3d4s$ ,  $3d4p$ ,  $4s4p$ ,  $3d4d$ , and  $3d4f$ . Many lines in Ca I, Ti III, Cr V, Mn VI, Fe VII, and Ni IX observed in the solar spectra have been identified in works such as [24, 25]. Resonance transitions in Co VIII, Ni IX and Cu X have been analyzed as well as the energies and weighted oscillator strengths have been calculated for Co VIII by Fawcett et al. [26]. The E1, M1, and M2 transition probabilities of some transitions in Ti III and V IV have been calculated using the orthogonal operator method by Raassen and Uylings [27]. Safronova et al. [28, 29] have used the relativistic many-body perturbation theory (RMBPT) to calculate the excitation energies and radiative rates of Ca-like ions. the calculated

spectra are arising from E2 and M1 transitions. Observed wavelengths of the  $3d4p \rightarrow 3d4d$  and  $3d4d \rightarrow 3d4f$  transitions in the vacuum ultraviolet spectra of calcium-like Mn VI, Fe VII and Co VIII have been identified [30], the MCHF method and isoelectronic comparison have been used for the classification.

The forbidden transitions E2, M1 have been studied using three different methods (MCDF, HFR, and SST), transition probabilities and oscillator strengths in Ca-like Ti III have been computed [31]. Oscillator strengths have been calculated for transitions between the  $3d^2$ ,  $3p^5 3d^3$ ,  $3d4p$ ,  $3d4f$  levels in Ca-like iron, cobalt and nickel using the pseudo-relativistic Hartree-Fock (HFR), the calculated results are reported in Ref. [20]. Recently, observed values of oscillator strengths of Ca I have been reported by Haq *et al.* [32] using the thermionic diode ion detector in conjunction with a Nd:YAG pumped dye laser system. The spectrum of Cu X has been studied using high-resolution vacuum spectrographs, and the excited energies of the  $3d^2$ ,  $3p^5 3d^3$ ,  $3d4p$ ,  $3d4f$  levels have been determined using the HF method [33]. Zhang *et al.* [34] calculated oscillator strengths and transition probabilities of Ti III using the weakest bound electron potential model (WBEPM). The calcium like titanium has been studied again [35] where, the oscillator strengths and radiative rates have been computed using the CIV3 program. The energy levels and collision strengths of Sc II have been computed using R-matrix package, transitions arising from the  $3d4s$ ,  $3d^2$ ,  $4s^2$ ,  $3d4p$ ,  $4s4p$ ,  $3d5s$ ,  $3d4d$ ,  $3d5p$ ,  $4p^2$ , and  $3d4f$  configurations are included [36].

The early compilation of atomic data of Ca-like ions performed by Wiese *et al.* [37], and Smith and Wise [38]. Compiled results including ions belonging to calcium isoelectronic sequence have been presented by Morton [39], the transition probabilities and oscillator strengths of several lines in Ca I, Sc II, and Ti III are reported. Another compilations performed by Corlis and Sugar [40], and Sugar *et al.* [41–43] have reported energy levels of calcium through zinc. Fuhr *et al.* [44, 45] have compiled experimental and theoretical data for transition probabilities for iron through nickel. Another compilations of transition probabilities for scandium through manganese ions have been performed by Martin *et al.* [46], and for energy levels of all ionization stages of scandium by Kaufman and Sugar [47]. The compilation processes still go on where, Shirai *et al.* [48, 49] have collected experimental and theoretical results of energy levels, oscillator strengths, and transition probabilities of Cr V and Co VIII, and for Ca-like Ti through Cu in the published monograph [50]. Wavelengths, energy levels, level classifications, oscillator strengths, and radiative transition probabilities for the nickel ions Ni IX to Ni XXVIII have been collected by Shirai *et al.* [51].

From the previous review we can figure out that the calcium isoelectronic sequence has been widely studied, despite this a limited works have provided an extensive calculations of energies and radiative parameters of many ionic species in this sequence, but for most of ions we still lack abundance of atomic data, especially for nickel and zinc. In the present

study, the configuration interaction calculations for calcium isoelectronic sequence with atomic charge  $Z=22$  to 30 have been performed using the non-relativistic CIV3 code [52, 53], and Los Alamos atomic physics code (LANL) based on Cowan's method which publicly available via website (<http://aphysics2.lanl.gov/cgi-bin/ION/runlanl08d.pl>). The iron ion was excluded from the study. The configuration groups  $3d^2$ ,  $3d4s$ ,  $3d4p$ ,  $3d4d$ , and  $3d4f$  with different angular momenta ( $J$ ) and parities are included in the configuration state list.

## 2. The Choice of Wave Functions

The present calculations have been performed using the configuration interaction method (CIV3 code) including relativistic effects of Hibbert [52, 53]. The LS states belonging to configurations of Ca-like Ti III to

Zn XI give 63 fine structure level, and about 150 or more up to 227 transitions between levels corresponding to various  $J$  values (in this paper we mentioned for examples about 40 transitions). All intermediate coupling (LS-coupling) atomic states under consideration are expressed as linear combinations of configuration wave functions in the form:

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

The single configuration wave functions  $\phi_i$  are consist of one electron functions.  $\alpha_{i,LS}$  defines the coupling of angular momenta to form a total  $L$  and  $S$  common to all configurations in Eq 1. The CIV3 method theory has been described in details in many previous works, for example Refs. [52–62]. In the present calculations the  $1s$ ,  $2s$ ,  $2p$ ,  $3s$ ,  $3p$  and  $3d$  radial functions are taken as the Hartree-Fock orbitals of the ground state  $3p^6 3d^2$  of Ca-like ions as given by Clementi and Roetti [63]. The other radial functions for  $4l$  are chosen as a spectroscopic type and are optimized using the CIV3 program [52]. The  $5s$ ,  $5p$ ,  $5d$ , and  $5f$ ,  $6s$ - $6f$  orbitals are chosen as a correlation orbitals (contributions from higher order levels with  $n + 2$  to improve the wave functions of the spectroscopic orbitals). The oscillator strengths in length and velocity gauge forms are given by:

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

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

The LANL atomic code based on Cowan method is described in details in Ref. [64]. Extensive configuration-interaction (CI) wave functions in intermediate coupling scheme have been generated. Despite that, the produced results are in LSJ-coupling, the intermediate  $LS$  coupling configuration state list is successfully effective in the evaluation of the Hamiltonian matrix elements [65, 66]. These wave functions are used to calculate the excitation energies, oscillator strengths and transition probabilities for allowed electric-dipole and intercombination transitions among the states of Ca-like ions with  $22 \leq Z \leq 30$ .

**Table 1.** Energy levels of Ca-like Ti III and V IV.

		Ti III			V IV			
Index	Level	Term	LANL	CIV3	NIST	LANL	CIV3	NIST
1	3d <sup>2</sup>	<sup>3</sup> F <sub>2</sub>	0	0	0	0	0	0
2		<sup>3</sup> F <sub>3</sub>	194.59	182.9	184.9	331.75	316.73	325.4
3		<sup>3</sup> F <sub>4</sub>	447.19	423.03	420.4	758.71	732.87	734.7
4		<sup>1</sup> D <sub>2</sub>	9049.5	8781.64	8473.5	11625	11069.39	10959.3
5		<sup>3</sup> P <sub>0</sub>	10923	10519.8	10538	13687	12994.95	13122.8
6		<sup>3</sup> P <sub>1</sub>	10991	10581.46	10604	13804	13101.02	13239.2
7		<sup>3</sup> P <sub>2</sub>	11134	10706.07	10721	14059	13287.89	13458.3
8		<sup>1</sup> G <sub>4</sub>	14170	14050.72	14398	17897	17534.39	18391.2
9		<sup>1</sup> S <sub>0</sub>	33786	32973.27	32476	42920	41754.26	42462.1
10	3d4p	<sup>1</sup> D <sub>2</sub>	73975	75255.85	75198	144130	144103.62	144273.1
11		<sup>3</sup> D <sub>1</sub>	75174	77289.25	77000	145340	146211.58	146117.7
12		<sup>3</sup> D <sub>2</sub>	75362	77330.2	77167	145660	146373.9	146429.3
13		<sup>3</sup> D <sub>3</sub>	75608	77444.78	77424	146060	146614.52	146855.1
14		<sup>3</sup> F <sub>2</sub>	75840	77466.03	77422	146490	147094.32	147135.2
15		<sup>3</sup> F <sub>3</sub>	76116	77607.81	77746	146940	147272.85	147656.5
16		<sup>3</sup> F <sub>4</sub>	76503	77658.11	78159	147590	147512.76	148369.2
17		<sup>3</sup> P <sub>0</sub>	78937	80967.72	80945	150350	151321.82	151449.1
18		<sup>3</sup> P <sub>1</sub>	78959	81069.84	80939	150360	151485.42	151427
19	3d4d	<sup>3</sup> P <sub>2</sub>	79072	81287.24	81024	150540	151818.24	151567.3
20		<sup>1</sup> F <sub>3</sub>	80824	84265.47	83117	152370	155088.17	153918.7
21		<sup>1</sup> P <sub>1</sub>	82241	81069.84	83797	154310	157289.38	155565.5
22		<sup>1</sup> F <sub>3</sub>	124300	129425.9	127791	213540	216896.02	215957.7
23		<sup>3</sup> D <sub>1</sub>	124790	129757	128433	214280	217816.48	216905
24		<sup>3</sup> D <sub>2</sub>	124910	129823	128546	214470	217924.32	217108
25		<sup>3</sup> D <sub>3</sub>	125050	129922	128690	214710	218086.29	217350
26		<sup>3</sup> G <sub>3</sub>	125320	130127.9	129093	215060	218684.65	217836.3
27		<sup>3</sup> G <sub>4</sub>	125480	130259.9	129253	215320	218900.37	218100
28	3d4f	<sup>3</sup> G <sub>5</sub>	125700	130425.1	129469	215670	219170.61	218463.6
29		<sup>1</sup> P <sub>1</sub>	125620	129823	129253	215520	219011.68	217990.7
30		<sup>3</sup> S <sub>1</sub>	126820	131202.7	130740	217380	221169.09	220343.5
31		<sup>1</sup> D <sub>2</sub>	136100	134413.7	135405	227320	226146.02	225804.1
32		<sup>3</sup> P <sub>0</sub>	136620	134863.2	135541	228110	226763.72	226521.6
33		<sup>3</sup> P <sub>1</sub>	136670	134896	135601	228210	226816.35	226617.1
34		<sup>3</sup> P <sub>2</sub>	136780	134977.5	135722	228380	226918.72	226796.3
35		<sup>1</sup> G <sub>4</sub>	137220	134275.7	136340	228970	227461.36	227712.5
36		<sup>1</sup> S <sub>0</sub>	141430	136611.8	140019	234710	238887.5	234121.8
37	3d4f	<sup>1</sup> G <sub>4</sub>	155950	159671.5	158285	261320	259873.08	263111.4
38		<sup>3</sup> F <sub>2</sub>	156180	159684.3	158537	261760	261448.24	263593
39		<sup>3</sup> F <sub>3</sub>	156190	159732.5	158558	261830	261514.7	263608.3
40		<sup>3</sup> F <sub>4</sub>	156320	159796.9	158691	262010	261603.98	264113.1

### 3. Results and Discussions

#### 3.1. Energy Levels

The calculated values of energies of 40 fine structure levels of Ca-like ions ( $Z = 22 - 30$ ) are listed in Tables 1-3 the data of iron ion have been excluded because we believe that we will not provide any significant results more than hitherto published. The present energies from CIV3 and LANL codes have been arranged in ascending order and

compared with the energy values taken from NIST atomic database [67]. The comparisons show good agreement with those in the literature, where the deviations from the values of NIST are better than 1.0% for most calculated levels. The cited values by NIST [67] are primarily taken from the compiled experimental and theoretical results by Sugar and Corliss [41] for Ca-like Ti III– Ni IX ions, from [42] for Cu X, and from [43] for Zn XI.

**Table 2.** Energy levels of Ca-like Cr V, Mn VI and Co VIII.

Index	Level	Term	Cr V			Mn VI			Co VII		
			LANL	CIV3	NIST	LANL	CIV3	NIST	LANL	CIV3	NIST
1	3d <sup>2</sup>	<sup>3</sup> F <sub>2</sub>	0	0	0	0	0	0	0	0	0
2		<sup>3</sup> F <sub>3</sub>	513.4	484.17	508.2	749.24	711.28	746	1426.3	1420.64	1430
3		<sup>3</sup> F <sub>4</sub>	1167.6	1120.47	1141.7	1693.4	1647.03	1669	3177.8	3291.94	3144
4		<sup>1</sup> D <sub>2</sub>	13924	12946.3	13188	16134	14905.23	15336	20537	20181.34	19624
5		<sup>3</sup> P <sub>0</sub>	16236	15042.46	15491.8	18665	17113.28	17782	23406	22683.42	22304
6		<sup>3</sup> P <sub>1</sub>	16419	15204.17	15676.6	18937	17351.22	18057	23944	23160.62	22839
7		<sup>3</sup> P <sub>2</sub>	16830	15490.82	16041	19559	17776.67	18628	25219	24022.64	24055
8		<sup>1</sup> G <sub>4</sub>	21379	21160.7	22019.2	24720	24988.51	25511	31367	30257.95	32360
9		<sup>1</sup> S <sub>0</sub>	51460	49304.46	51146.4	59361	56819.76	59265	74667	71654.49	74247
10	3d4p	<sup>1</sup> D <sub>2</sub>	227050	225814.5	226119.8	321800	319083.1	319821	545380	538332	542430
11		<sup>3</sup> D <sub>1</sub>	228290	228148.1	228001.8	323090	321519.1	321694	546830	541105.5	542701
12		<sup>3</sup> D <sub>2</sub>	228790	228397.1	228489.1	323820	321891.7	322410	548270	541825.6	544314
13		<sup>3</sup> D <sub>3</sub>	229380	228765.9	229120.8	324640	322443.9	323283	549590	542893	545834
14		<sup>3</sup> F <sub>2</sub>	229830	229804.9	229551.7	325010	323950.7	323796	549660	544317.6	547400
15		<sup>3</sup> F <sub>3</sub>	230510	230081.8	230316.3	325960	324369.7	324849	551280	545113.9	548799
16		<sup>3</sup> F <sub>4</sub>	231500	230453.9	231392.9	327380	324932.4	326373	553780	546184.4	551524
17		<sup>3</sup> P <sub>0</sub>	234520	235043.9	234668.5	330590	330093.1	329729	557070	552120.1	549153.1
18		<sup>3</sup> P <sub>1</sub>	234510	235291	234618.4	330540	330457.7	329635	556860	552840.3	549634.9
19	3d4d	<sup>3</sup> P <sub>2</sub>	234790	235794.1	234846.4	330960	331199.4	329992	557780	554307.5	551248.9
20		<sup>1</sup> F <sub>3</sub>	236890	239661.2	237529.5	333290	335394.1	333055	560570	559452.3	557736
21		<sup>1</sup> P <sub>1</sub>	239410	242835.7	239917.5	336340	339462.2	336131	564760	564772.7	563271
22		<sup>1</sup> F <sub>3</sub>	315590	317266	316674.9	428990	428995	429105	689550	693978.6	—
23		<sup>3</sup> D <sub>1</sub>	316480	318315.5	317893.8	430070	431447.9	429105	690890	696773.5	—
24		<sup>3</sup> D <sub>2</sub>	316790	318490.8	318227.6	430520	431739.6	431059	691800	697350.9	—
25		<sup>3</sup> D <sub>3</sub>	317160	318754.1	318601.7	431060	432177.8	431607	692990	698219.2	—
26		<sup>3</sup> G <sub>3</sub>	317480	319313.9	319119.1	431340	433026.2	432091	692600	699375.3	—
27		<sup>3</sup> G <sub>4</sub>	317860	319663.9	319516.8	431870	433608.1	432653	693700	700534	—
28	3d4f	<sup>3</sup> G <sub>5</sub>	318410	320102.3	320074.4	432660	434337.4	433464	695190	701987.4	—
29		<sup>1</sup> P <sub>1</sub>	318140	319808.7	319284	432250	433780.1	436451	694360	700807.7	—
30		<sup>3</sup> S <sub>1</sub>	320570	322443.9	322528.1	435350	438207.8	436451	698830	708820	—
31		<sup>1</sup> D <sub>2</sub>	332210	329232.1	329350.3	448430	451241.7	444637	714820	732765.1	—
32		<sup>3</sup> P <sub>0</sub>	333110	329906.6	330084.8	449450	452170.7	452173.7	716020	734726.6	—
33		<sup>3</sup> P <sub>1</sub>	333250	329990.2	330245.1	449670	452307	445591	716470	735014.4	—
34		<sup>3</sup> P <sub>2</sub>	333530	330150.7	330536.8	450090	452562.8	446044	717330	735539.2	—
35		<sup>1</sup> G <sub>4</sub>	334440	333215.1	331811.2	451180	443481.3	447702	718720	739418.4	—
36		<sup>1</sup> S <sub>0</sub>	343460	336956.7	—	462230	449183.5	—	733990	765972.9	—
37	3d4f	<sup>1</sup> G <sub>4</sub>	380420	381453.4	—	511690	509423.6	518905	808340	808844.6	811205
38		<sup>3</sup> F <sub>2</sub>	381120	382358.2	—	512730	510090.7	501976	810200	809975.1	812862
39		<sup>3</sup> F <sub>3</sub>	381250	382463.7	—	512950	510251.1	502639	810640	810285.2	813298
40		<sup>3</sup> F <sub>4</sub>	381670	382605.1	—	513460	510465.6	503432	811530	810700.4	814130

Ti III: The calculated values of energy levels of Ti III have been listed in Table 1 and agree well with the corresponding values of NIST [67], and the maximum deviation was found for the 3d<sup>2</sup> <sup>1</sup>D<sub>2</sub> level by value of 3.64% from the corresponding value by NIST (for the calculations using CIV3). For the calculations using the LANL code the maximum deviations from NIST values are recorded for the 3d<sup>2</sup> <sup>3</sup>F<sub>3,4</sub> and <sup>1</sup>D<sub>2</sub> levels with deviations of 5.24, 6.37, 6.8%, respectively. For this ion, it is clear that the calculations using

CIV3 are better than those using LANL code.

V IV: When we compared the energies of the calcium-like vanadium (Z = 24) with the compiled results by NIST, we found that most of calculated results show good agreement with those from NIST. The maximum deviation was found for the 3d<sup>2</sup> <sup>1</sup>G<sub>4</sub> level by a value of 4.66% for the CIV3 calculations and for the 3d<sup>2</sup> <sup>1</sup>D<sub>2</sub> level by a value of 6.1% using the LANL calculations, This data has been listed in Table 1.

**Table 3.** Energy levels of Ca-like Ni IX, Cu X and Zn XI.

Index	Level	Term	Ni IX			Cu X			Zn XI		
			LANL	CIV3	NIST	LANL	CIV3	NIST	LANL	CIV3	NIST
1	3d <sup>2</sup>	<sup>3</sup> F <sub>2</sub>	0	0	0	0	0	0	0	0	0
2		<sup>3</sup> F <sub>3</sub>	1891.6	1821.22	1880	2459.9	2493.04	2486	3146.3	1802.02	1890
3		<sup>3</sup> F <sub>4</sub>	4180.7	4221.67	4070	5389.9	5782.31	5487	6830.8	4164.41	4120
4		<sup>1</sup> D <sub>2</sub>	22783	22397.88	21900	25084	24934.14	23900	27459	25581.16	26070
5		<sup>3</sup> P <sub>0</sub>	25770	24885.52	—	28154	27284.57	—	30567	28643.85	—
6		<sup>3</sup> P <sub>1</sub>	26499	25497.8	—	29122	28122.37	—	31836	29255.31	—
7		<sup>3</sup> P <sub>2</sub>	28248	26608.75	27160	31468	29656.87	30600	34919	30309.36	31330
8		<sup>1</sup> G <sub>4</sub>	34761	36858.31	35898	38248	36824.33	—	41858	38470.6	—
9		<sup>1</sup> S <sub>0</sub>	82256	82796.39	—	89881	85995.92	—	97592	103377.4	—
10	3d4p	<sup>1</sup> D <sub>2</sub>	673780	680134.9	—	812950	817112.7	—	962920	876844	—
11		<sup>3</sup> D <sub>1</sub>	675370	681778.2	—	814750	819251.9	—	964980	879297.6	—
12		<sup>3</sup> D <sub>2</sub>	677310	682776.9	—	817310	820567.8	—	968310	880165.2	—
13		<sup>3</sup> D <sub>3</sub>	678870	684262.3	—	819080	822522.9	—	970260	881448.1	—
14		<sup>3</sup> F <sub>2</sub>	678820	685948.3	—	818970	823452.7	—	970190	882384.1	—
15		<sup>3</sup> F <sub>3</sub>	680850	687104.3	—	821490	824944.5	—	973240	883149.2	—
16		<sup>3</sup> F <sub>4</sub>	684000	688653.6	—	825340	826946.1	—	977890	884186.1	—
17		<sup>3</sup> P <sub>0</sub>	687140	693169.9	—	828200	832064.7	—	980290	888968.4	—
18		<sup>3</sup> P <sub>1</sub>	686820	694111.4	—	827710	833340.4	—	979610	890080.7	—
19	3d4d	<sup>3</sup> P <sub>2</sub>	688120	696015.4	—	829520	835928.9	—	982060	892358.5	—
20		<sup>1</sup> F <sub>3</sub>	691130	699267.3	—	832730	840677.6	—	985440	896638.7	—
21		<sup>1</sup> P <sub>1</sub>	695940	704670.5	—	838230	846928.1	—	991680	901391.8	—
22		<sup>1</sup> F <sub>3</sub>	836440	841290.5	—	994170	992064.6	—	1162800	1079148	—
23		<sup>3</sup> D <sub>1</sub>	837850	843968.1	—	995600	994627	—	1164200	1081443	—
24		<sup>3</sup> D <sub>2</sub>	839090	844714.8	—	997240	995612.4	—	1166400	1082142	—
25		<sup>3</sup> D <sub>3</sub>	840650	845837.5	—	999280	997093.7	—	1169000	1083191	—
26		<sup>3</sup> G <sub>3</sub>	839890	846521.4	—	997990	997163.4	—	1167000	1083737	—
27		<sup>3</sup> G <sub>4</sub>	841260	848019.5	—	999700	999140.2	—	1169100	1085138	—
28	3d4f	<sup>3</sup> G <sub>5</sub>	843230	849898.2	—	1002200	1001618	—	1172300	1086896	—
29		<sup>1</sup> P <sub>1</sub>	842110	848383.2	—	1000800	999631.9	—	1170400	1085579	—
30		<sup>3</sup> S <sub>1</sub>	847270	856674.7	—	1006600	1008474	—	1177000	1092758	—
31		<sup>1</sup> D <sub>2</sub>	864590	877850.7	—	1025300	1029314	—	1196900	1106593	—
32		<sup>3</sup> P <sub>0</sub>	865840	879761.5	—	1026500	1031236	—	1198200	1108634	—
33		<sup>3</sup> P <sub>1</sub>	866460	880139.1	—	1027400	1031737	—	1199300	1108995	—
34		<sup>3</sup> P <sub>2</sub>	867630	880839	—	1028900	1032674	—	1201300	1109663	—
35		<sup>1</sup> G <sub>4</sub>	869110	862780	—	1030500	1036387	—	1202800	1138016	—
36		<sup>1</sup> S <sub>0</sub>	886500	871851.1	—	1050000	1063559	—	1224600	1131073	—
37	3d4f	<sup>1</sup> G <sub>4</sub>	973200	974774.3	—	1148800	1132341	—	1335100	1242394	—
38		<sup>3</sup> F <sub>2</sub>	975520	976313.7	977130	1151600	1136300	—	1338400	1249097	—
39		<sup>3</sup> F <sub>3</sub>	976120	976724.5	977680	1152400	1136798	—	1339400	1249372	—
40		<sup>3</sup> F <sub>4</sub>	977290	977274.8	978740	1153900	1137469	—	1341400	1249751	—

Cr V: In the Cr IV ion the 3d<sup>2</sup> <sup>3</sup>F<sub>3</sub> level deviates from the corresponding NIST value by 4.73% for the CIV3 and the value of 5.6% is recorded as a deviation of the 3d<sup>2</sup> <sup>1</sup>D<sub>2</sub> level from NIST value for the LANL calculations, the value of energy levels have been listed in Table 2.

Mn VI: The same as Cr IV was figured out for the Mn ion where, the 3d<sup>2</sup> <sup>3</sup>F<sub>3</sub> level deviates from the corresponding NIST value by 4.65% for the CIV3 and the value of 5.2% is recorded as a deviation of the 3d<sup>2</sup> <sup>1</sup>D<sub>2</sub> level from NIST value for the LANL calculations, as shown in Table 2.

Co VIII: For most of levels calculated using CIV3 the energies agree well with those from NIST and the percent

differences are less than 1.0%, except the 3d<sup>2</sup> <sup>1</sup>G<sub>4</sub> where the deviation rises to 6.0%. The maximum deviations for the results produced by LANL are 4.9, 4.8, 4.8% for 3d<sup>2</sup> <sup>3</sup>P<sub>0,1,2</sub>, respectively, as shown in Table 2.

Ni IX: The ground state and excitation energies of Ca-like Ni IX are shown in Table 3, the data have been compared with the minor ones available by NIST atomic spectra database [67], and it is in a reasonable agreement with the literature [67]. But in some cases this agreement disappears for example, the levels 3d<sup>2</sup> <sup>1</sup>D<sub>2</sub> and 3d<sup>2</sup> <sup>3</sup>F<sub>3,4</sub> which showing differences from NIST by 4.0, 3.1, 3.7%, respectively.

**Table 4.** Oscillator strengths, wavelengths, and transition probabilities for Ca-like Co VIII.

Index	UL.	LL.	$\lambda$	$f_L$	$f_V$	$f_{LANL}$	$A_L$	$L/V$
1	$3d^2(^3F_2)$	$3d4p(^3D_1)$	184.81	6.91E-02	7.50E-02	7.90E-02	2.25E+10	0.92
2		$3d4p(^3D_2)$	184.56	1.28E-02	1.39E-02	1.90E-02	2.51E+09	0.92
3		$3d4p(^3D_3)$	184.2	3.67E-04	3.95E-04	2.43E-03	5.15E+07	0.93
4		$3d4p(^3F_2)$	183.72	3.68E-02	3.94E-02	2.29E-02	7.27E+09	0.93
5		$3d4p(^3F_3)$	183.45	4.61E-03	4.92E-03	3.46E-03	6.52E+08	0.94
6		$3d4f(^3F_2)$	123.46	8.21E-02	8.70E-02	1.46E-01	3.59E+10	0.94
7		$3d4f(^3F_3)$	123.41	1.03E-02	1.09E-02	6.35E-02	3.21E+09	0.94
8		$3d4f(^3G_3)$	122.97	2.81E-01	2.76E-01	5.39E-01	8.85E+10	1.02
9		$3d4f(^3D_1)$	122.7	6.30E-03	6.16E-03	1.34E-02	4.65E+09	1.02
10		$3d4f(^3D_2)$	122.7	1.17E-03	1.14E-03	1.12E-03	5.17E+08	1.02
11		$3d4f(^3D_3)$	122.71	3.34E-05	3.27E-05	1.54E-02	1.06E+07	1.02
12	$3d^2(^3F_3)$	$3d4p(^3D_2)$	185.05	7.34E-02	7.94E-02	7.10E-02	2.00E+10	0.92
13		$3d4p(^3D_3)$	184.68	9.19E-03	9.90E-03	3.27E-02	1.80E+09	0.93
14		$3d4p(^3F_2)$	184.2	3.29E-03	3.53E-03	1.60E-02	9.06E+08	0.93
15		$3d4p(^3F_3)$	183.93	3.49E-02	3.73E-02	1.97E-02	6.88E+09	0.94
16		$3d4p(^3F_4)$	183.57	3.34E-03	3.56E-03	4.05E-03	5.15E+08	0.94
17		$3d4f(^3D_2)$	122.91	6.66E-03	6.54E-03	1.59E-02	4.12E+09	1.02
18		$3d4f(^3D_3)$	122.92	8.34E-04	8.19E-04	5.19E-03	3.68E+08	1.02
19		$3d4f(^3G_3)$	123.19	1.75E-02	1.73E-02	5.56E-02	7.71E+09	1.01
20		$3d4f(^3G_4)$	123.1	2.63E-01	2.59E-01	5.14E-01	9.02E+10	1.02
21		$3d4f(^3F_2)$	123.68	7.32E-03	7.79E-03	9.71E-03	4.47E+09	0.94
22		$3d4f(^3F_3)$	123.63	7.76E-02	8.25E-02	1.16E-01	3.39E+10	0.94
23		$3d4f(^3F_4)$	123.57	7.44E-03	7.90E-03	3.61E-02	2.53E+09	0.94
24	$3d^2(^3F_4)$	$3d4p(^3D_3)$	185.32	8.29E-02	8.93E-02	6.38E-02	2.07E+10	0.93
25		$3d4p(^3F_3)$	184.56	2.60E-03	2.78E-03	3.39E-02	6.55E+08	0.94
26		$3d4p(^3F_4)$	184.2	3.91E-02	4.16E-02	4.70E-02	7.69E+09	0.94
27		$3d4f(^3F_4)$	123.85	8.67E-02	9.25E-02	1.19E-01	3.77E+10	0.94
28		$3d4f(^3F_3)$	123.92	5.77E-03	6.16E-03	6.19E-03	3.22E+09	0.94
29		$3d4f(^3G_3)$	123.47	2.16E-04	2.14E-04	3.54E-04	1.22E+08	1.01
30		$3d4f(^3G_4)$	123.38	1.36E-02	1.35E-02	5.43E-02	5.98E+09	1.01
31		$3d4f(^3G_5)$	123.27	2.67E-01	2.64E-01	5.67E-01	9.60E+10	1.01
32		$3d4f(^3D_3)$	123.2	7.49E-03	7.39E-03	1.59E-02	4.23E+09	1.01
33		$3d4p(^3D_1)$	192.89	3.19E-02	3.41E-02	4.52E-02	1.90E+09	0.93
34		$3d4p(^3P_1)$	188.62	9.77E-02	1.00E-01	9.78E-02	6.10E+09	0.98
35	$3d^2(^3P_0)$	$3d4f(^3D_1)$	126.21	2.47E-01	2.48E-01	7.02E-01	3.45E+10	0.99
36		$3d4f(^3P_1)$	125.99	1.25E-01	1.26E-01	9.44E-02	1.76E+10	0.99
37		$3d4p(^3D_1)$	193.07	7.97E-03	8.53E-03	6.30E-03	1.43E+09	0.93
38		$3d4p(^3D_2)$	192.8	2.39E-02	2.56E-02	3.25E-02	2.58E+09	0.94
39		$3d4p(^3P_1)$	188.79	2.44E-02	2.50E-02	3.02E-02	4.57E+09	0.98
40		$3d4p(^3P_0)$	189.05	3.25E-02	3.34E-02	3.82E-02	1.82E+10	0.97

**Table 5.** Oscillator strengths, wavelengths, and transition probabilities for Ca-like Ni IX.

Index	UL.	LL.	$\lambda$	$f_L$	$f_V$	$f_{LANL}$	$A_L$	$L/V$
1	$3d^2(^3F_2)$	$3d4p(^3D_1)$	146.68	5.87E-02	5.31E-02	7.36E-02	3.03E+10	1.11
2		$3d4p(^3D_2)$	146.46	1.09E-02	9.82E-03	1.69E-02	3.39E+09	1.11
3		$3d4p(^3D_3)$	146.14	3.12E-04	2.80E-04	2.79E-03	6.95E+07	1.11
4		$3d4p(^3F_2)$	145.78	3.12E-02	2.79E-02	1.76E-02	9.81E+09	1.12
5		$3d4p(^3F_3)$	145.54	3.91E-03	3.49E-03	2.71E-03	8.80E+08	1.12
6		$3d4f(^3G_3)$	101.92	3.16E-01	3.40E-01	6.08E-01	1.45E+11	0.93
7		$3d4f(^3D_1)$	101.7	7.08E-03	7.58E-03	1.48E-02	7.61E+09	0.93
8		$3d4f(^3D_3)$	101.71	3.75E-05	4.02E-05	1.75E-02	1.73E+07	0.93
9	$3d^2(^3F_3)$	$3d4p(^3D_2)$	146.85	6.24E-02	5.62E-02	6.44E-02	2.70E+10	1.11
10		$3d4p(^3D_3)$	146.53	7.81E-03	7.01E-03	3.54E-02	2.43E+09	1.11
11		$3d4p(^3F_2)$	146.17	2.80E-03	2.50E-03	1.68E-02	1.22E+09	1.12
12		$3d4p(^3F_3)$	145.93	2.97E-02	2.64E-02	1.38E-02	9.29E+09	1.12
13		$3d4p(^3F_4)$	145.6	2.84E-03	2.52E-03	3.81E-03	6.96E+08	1.13
14		$3d4f(^3D_2)$	101.89	7.49E-03	8.05E-03	1.72E-02	6.74E+09	0.93
15		$3d4f(^3D_3)$	101.9	9.38E-04	1.01E-03	6.10E-03	6.03E+08	0.93
16		$3d4f(^3G_3)$	102.11	1.97E-02	2.13E-02	6.13E-02	1.26E+10	0.93
17	$3d^2(^3F_4)$	$3d4f(^3G_4)$	102.03	2.96E-01	3.19E-01	5.80E-01	1.48E+11	0.93
18		$3d4p(^3D_3)$	147.05	7.05E-02	6.32E-02	5.01E-02	2.80E+10	1.12
19		$3d4p(^3F_3)$	146.44	2.21E-03	1.97E-03	4.11E-02	8.85E+08	1.12
20		$3d4p(^3F_4)$	146.11	3.33E-02	2.94E-02	4.42E-02	1.04E+10	1.13
21		$3d4f(^3G_3)$	102.36	2.43E-04	2.63E-04	3.19E-04	1.99E+08	0.92
22		$3d4f(^3G_4)$	102.28	1.54E-02	1.66E-02	6.06E-02	9.79E+09	0.92
23		$3d4f(^3G_5)$	102.17	3.01E-01	3.25E-01	6.39E-01	1.57E+11	0.93
24		$3d4f(^3D_3)$	102.15	8.44E-03	9.10E-03	1.88E-02	6.93E+09	0.93
25	$3d^2(^3P_0)$	$3d4p(^3D_1)$	152.23	2.72E-02	2.42E-02	4.46E-02	2.61E+09	1.12
26		$3d4p(^3P_1)$	149.43	8.30E-02	7.11E-02	8.84E-02	8.27E+09	1.17
27		$3d4f(^3D_1)$	104.34	2.74E-01	3.04E-01	8.00E-01	5.61E+10	0.9
28		$3d4f(^3P_1)$	104.19	1.40E-01	1.55E-01	9.15E-02	2.86E+10	0.9
29		$3d4p(^3D_1)$	152.38	6.80E-03	6.04E-03	5.48E-03	1.95E+09	1.12
30		$3d4p(^3D_2)$	152.14	2.04E-02	1.81E-02	3.18E-02	3.53E+09	1.13
31		$3d4p(^3P_1)$	149.56	2.08E-02	1.78E-02	2.87E-02	6.19E+09	1.17
32		$3d4p(^3P_0)$	149.78	2.77E-02	2.38E-02	3.59E-02	2.47E+10	1.16
33	$3d^2(^3P_2)$	$3d4p(^3P_2)$	149.14	3.47E-02	2.96E-02	3.66E-02	6.25E+09	1.17
34		$3d4f(^3D_1)$	104.41	6.86E-02	7.60E-02	8.75E-02	4.20E+10	0.9
35		$3d4f(^3D_2)$	104.41	2.06E-01	2.28E-01	5.60E-01	7.56E+10	0.9
36		$3d4f(^3P_1)$	104.25	3.49E-02	3.88E-02	1.39E-01	2.14E+10	0.9
37		$3d4f(^3P_0)$	104.18	4.65E-02	5.16E-02	9.97E-02	8.58E+10	0.9
38		$3d4p(^3P_1)$	149.81	2.08E-02	1.78E-02	1.76E-02	1.03E+10	1.17
39		$3d4p(^3P_2)$	149.39	6.26E-02	5.33E-02	8.15E-02	1.87E+10	1.17
40		$3d4p(^3D_2)$	152.4	4.09E-03	3.62E-03	2.58E-03	1.17E+09	1.13
41	$3d4p(^3D_1)$	$3d4d(^3F_2)$	546.64	3.99E-01	3.38E-01	5.52E-01	5.34E+09	1.18
42		$3d4d(^3P_0)$	505.1	3.85E-02	2.80E-02	7.20E-02	3.02E+09	1.37
43		$3d4d(^3P_1)$	504.14	2.89E-02	2.10E-02	2.35E-02	7.58E+08	1.38
44		$3d4d(^3D_2)$	613.74	5.57E-02	5.89E-02	6.44E-02	5.91E+08	0.95
45		$3d4d(^3D_1)$	616.57	1.66E-01	1.77E-01	2.60E-01	2.92E+09	0.94
46		$3d4d(^3F_2)$	549.64	4.41E-02	3.78E-02	7.96E-02	9.73E+08	1.17
47		$3d4d(^3F_3)$	546.3	3.55E-01	3.00E-01	4.21E-01	5.66E+09	1.18
48		$3d4d(^3P_1)$	506.69	5.18E-02	3.79E-02	9.65E-02	2.24E+09	1.36
49	$3d4p(^3D_2)$	$3d4d(^3P_2)$	504.9	1.73E-02	1.26E-02	1.34E-02	4.53E+08	1.37
50		$3d4d(^3D_1)$	620.39	3.30E-02	3.57E-02	3.21E-02	9.54E+08	0.93

**Table 6.** Oscillator strengths, wavelengths, and transition probabilities for Ca-like Cu X.

Index	UL.	LL.	$\lambda$	$f_L$	$f_V$	$f_{LANL}$	$A_L$	$L/V$
1	$3d^2(^3F_2)$	$3d4p(^3D_1)$	123.84	6.02E-02	6.12E-02	6.88E-02	4.36E+10	0.98
2		$3d4p(^3D_2)$	123.63	1.12E-02	1.13E-02	1.47E-02	4.87E+09	0.99
3		$3d4p(^3D_3)$	123.34	3.20E-04	3.23E-04	3.06E-03	1.00E+08	0.99
4		$3d4p(^3F_2)$	123.19	3.20E-02	3.22E-02	1.33E-02	1.41E+10	0.99
5		$3d4p(^3F_3)$	122.97	4.01E-03	4.02E-03	2.09E-03	1.26E+09	1
6	$3d^2(^3F_3)$	$3d4f(^3F_2)$	88.87	2.62E-01	2.37E-01	1.82E-01	2.21E+11	1.11
7		$3d4f(^3F_3)$	88.83	3.27E-02	2.96E-02	7.62E-02	1.98E+10	1.11
8		$3d4p(^3D_2)$	124.01	6.40E-02	6.48E-02	5.91E-02	3.88E+10	0.99
9		$3d4p(^3D_3)$	123.71	8.02E-03	8.08E-03	3.70E-02	3.49E+09	0.99
10		$3d4p(^3F_2)$	123.57	2.86E-03	2.88E-03	1.71E-02	1.75E+09	0.99
11	$3d^2(^3F_4)$	$3d4p(^3F_3)$	123.34	3.04E-02	3.05E-02	9.20E-03	1.33E+10	1
12		$3d4p(^3F_4)$	123.04	2.91E-03	2.91E-03	3.60E-03	9.98E+08	1
13		$3d4f(^3F_2)$	89.06	2.33E-02	2.12E-02	1.18E-02	2.75E+10	1.1
14		$3d4f(^3F_3)$	89.02	2.47E-01	2.24E-01	1.44E-01	2.08E+11	1.1
15		$3d4f(^3F_4)$	88.97	2.37E-02	2.15E-02	4.46E-02	1.55E+10	1.1
16	$3d^2(^3P_0)$	$3d4p(^3D_3)$	124.21	7.24E-02	7.29E-02	3.85E-02	4.02E+10	0.99
17		$3d4p(^3F_3)$	123.84	2.27E-03	2.27E-03	4.70E-02	1.27E+09	1
18		$3d4p(^3F_4)$	123.54	3.41E-02	3.40E-02	4.17E-02	1.49E+10	1
19		$3d4f(^3F_4)$	89.23	2.76E-01	2.51E-01	1.46E-01	2.31E+11	1.1
20		$3d4f(^3F_3)$	89.28	1.84E-02	1.67E-02	7.49E-03	1.98E+10	1.1
21	$3d^2(^3P_1)$	$3d4p(^3D_1)$	128.13	2.78E-02	2.77E-02	4.43E-02	3.76E+09	1
22		$3d4p(^3P_1)$	125.86	8.47E-02	8.17E-02	7.99E-02	1.19E+10	1.04
23		$3d4p(^3D_1)$	128.27	6.96E-03	6.94E-03	4.74E-03	2.82E+09	1
24		$3d4p(^3D_2)$	128.05	2.09E-02	2.08E-02	3.14E-02	5.10E+09	1.01
25		$3d4p(^3P_1)$	125.99	2.12E-02	2.04E-02	2.73E-02	8.90E+09	1.04
26	$3d^2(^3P_2)$	$3d4p(^3P_0)$	126.2	2.82E-02	2.73E-02	3.39E-02	3.54E+10	1.03
27		$3d4p(^3P_2)$	125.58	3.54E-02	3.39E-02	3.32E-02	8.99E+09	1.04
28		$3d4p(^3P_1)$	126.23	2.12E-02	2.05E-02	1.47E-02	1.48E+10	1.04
29		$3d4p(^3P_2)$	125.82	6.39E-02	6.12E-02	7.69E-02	2.69E+10	1.04
30		$3d4p(^3D_2)$	128.3	4.19E-03	4.16E-03	2.20E-03	1.70E+09	1.01
31	$3d^2(^1D_2)$	$3d4p(^3D_3)$	127.98	2.35E-02	2.32E-02	1.22E-02	6.84E+09	1.01
32		$3d4p(^1D_2)$	128.1	6.49E-02	6.47E-02	4.01E-02	2.64E+10	1
33		$3d4p(^1F_3)$	124.35	7.61E-03	7.18E-03	6.28E-03	2.34E+09	1.06
34		$3d4p(^1P_1)$	123.39	4.02E-02	3.74E-02	3.40E-02	2.94E+10	1.08
35		$3d4p(^1F_3)$	126.2	1.16E-01	1.08E-01	1.31E-01	6.24E+10	1.07
36	$3d^2(^1D_2)$	$3d4f(^1D_2)$	90.35	3.82E-01	3.44E-01	2.43E-01	3.12E+11	1.11
37		$3d4s(^3D_1)$	747.94	7.31E-02	6.58E-02	9.24E-02	2.62E+09	1.11
38		$3d4p(^3P_1)$	740.87	5.54E-02	4.89E-02	1.03E-01	6.73E+08	1.13
39		$3d4p(^3D_1)$	827.29	1.49E-01	1.64E-01	1.68E-01	1.45E+09	0.91
40		$3d4p(^3D_2)$	818.38	5.02E-02	5.40E-02	2.30E-02	3.00E+08	0.93

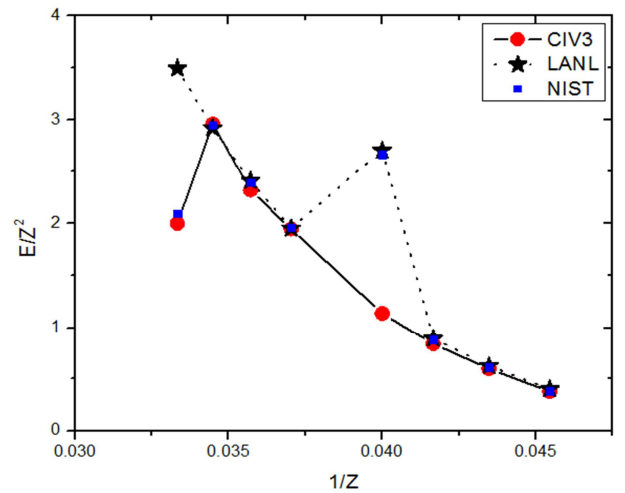
Cu X: The energy levels of Cu X have been listed in Table 3 and have been compared with the corresponding values of NIST. For the few available levels by NIST the comparisons show good agreement and the maximum deviation is found for the  $3d^2\ ^3F_4$  where the error value is about 5.38%.

Zn XI: The Zn XI data are tabulated in Table 3, it is clear that the computed energies using the CIV3 code are much more better than those computed using LANL, we can figure out this from the results deviations from NIST values. The deviation of the  $3d^2\ ^3F_3$  level is about 4.65% for the CIV3 calculations and about 66% for the LANL calculations. This worse deviation appears in the calculated values by LANL code is a little bit confuse us, because the Z-dependence of the calculated energies by LANL is fitting well with the formula [68]:

$$E = Z^2(E_0 + Z^{-1}E_1 + \dots) \quad (4)$$

Where, figures (1a-2b) show that, the NIST and CIV3 values of  $E/Z$  decrease systematically vs  $1/Z$  over all ions

except for zinc ion, while the calculations of LANL fit well with the equation (4) over all ions including Zn.

**Fig. 1a.** The Z-dependence of the  $3d^2\ ^3F_3$  energy level.



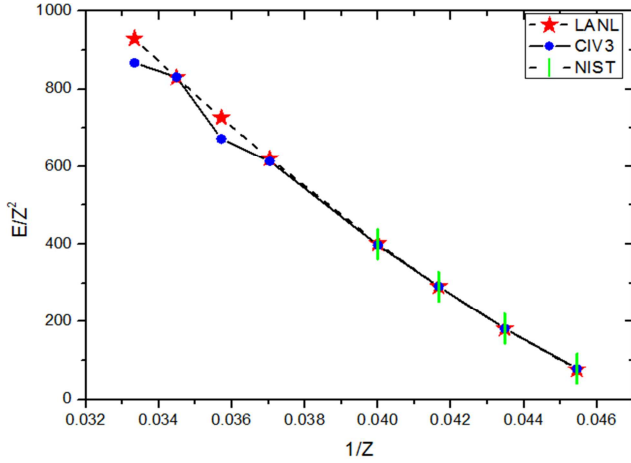


Fig. 1b. The Z-dependence of the  $3d4s\ ^3D_1$  energy level.

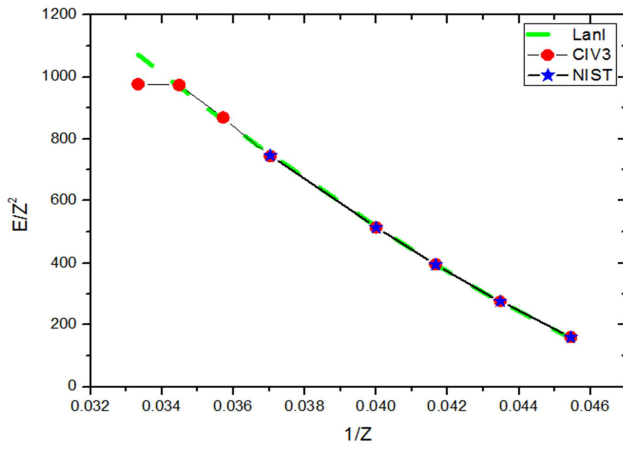


Fig. 2a. The Z-dependence of the  $3d4p\ ^3D_1$  energy level.

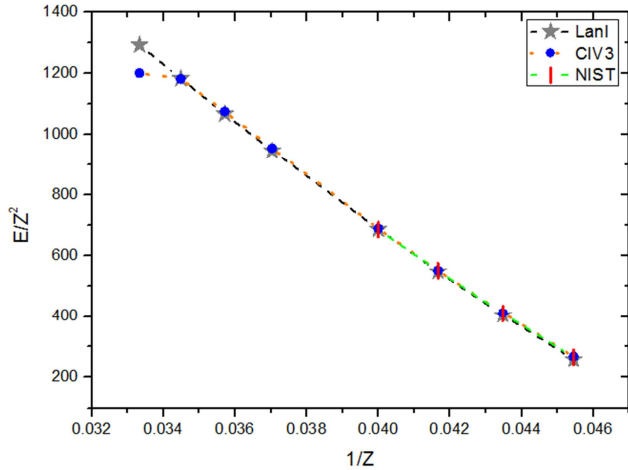


Fig. 2b. The Z-dependence of the  $3d4d\ ^3D_1$  energy level.

The fine structure parameter  $\zeta_i$  depend on the angular momentum  $l > 0$  and is given from:

$$H_{fs} = \sum_{i=1}^N \frac{\zeta_i}{r_i^3} l_i \cdot s_i. \quad (5)$$

Figure (3a) show that the CIV3 calculations of hyper fine structure parameter vary systematically with  $Z$ , except at Zn value which decreases rapidly. The  $\zeta_2/Z$  value was adjusted at 0.808 for the Zn ion to match the calculated energies by CIV3 with NIST, from the previous argument we think that the abnormal value of LANL calculations of the  $3d^2\ ^3F_3$  energy level in Zn XI are accurate and may be an error has been occurred in the compilation process for the zinc data in the literature [43].

### 3.2. Oscillator Strengths and Radiative Rates

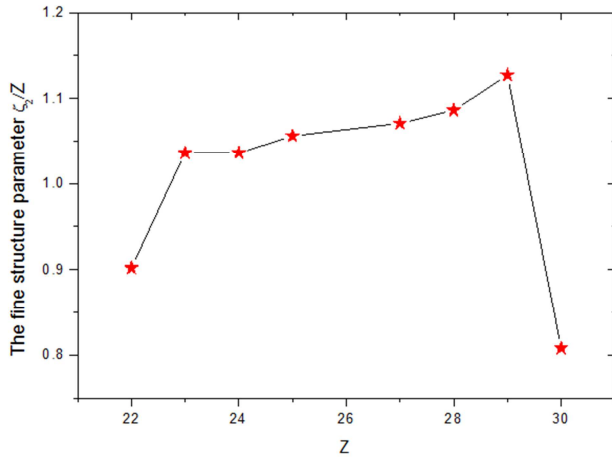
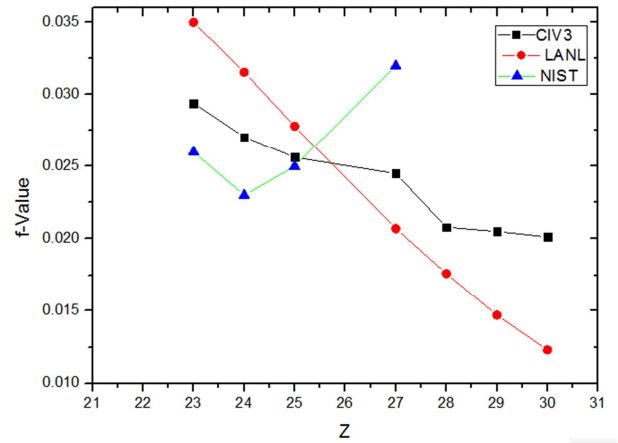
The configuration interaction calculations of radiative parameters (wavelengths, oscillator strengths, and transition probabilities) are given in Tables 4-7. In the present work, we have used two approximations to get better values for oscillator strengths and transition probabilities. First, the calculations using the non-relativistic configuration interaction method CIV3 including Breit-Pauli Hamiltonian. Second, the ab-initio calculations using the LANL atomic code based on Cowan's method [64]. It obvious that for the listed data of oscillator strengths, the data produced from CIV3 calculations are so close to those from LANL calculations for the majority of transitions.

The accuracy of the results could be estimated by many ways such as, the comparison with the previous published theoretical calculations and experimental data, the use of different methods in the calculations, and/or the convergence between the length and velocity gauge forms [69]. In the present work we have used two different methods in the calculations, and compared the calculated data of oscillator strengths from the two methods with the available sources, and checked the agreement between length and velocity gauge values. The comparisons between CIV3 and LANL calculations of oscillator strengths and other literature have been accomplished in Table 8. Where the present calculations have been compared with the values of NIST [67] as well as with the cited values in the literature [20, 26, 34, 44-46, 48, 49]. For most cited transitions in Table 8 our data either from CIV3 or from LANL are in a reasonable agreement with those of NIST and the literature, the deviation for some transitions reaches large values such as  $3d4p(^3D_3) - 3d4d(^3D_3)$  in V IV ion, which deviates from NIST by as much as 99% but the average deviation for this ion lies within 10%. To avoid worse accuracies like that we should include a large number of correlations within the used configuration state list using CIV3 by adding the  $7l$  and  $8l$  correlations. Procedure like this needs high speed computer containing large memory (not available for us at the present time).

An important point should be mentioned here, that is the accuracy (D, E) of most of NIST-values for oscillator strengths are about  $40\% \leq D \leq 50\%$  and  $E > 50\%$  which means that our calculated results of most oscillator strengths are in the uncertainty range of NIST.

**Table 7.** Oscillator strengths, wavelengths, and transition probabilities for Ca-like Zn XI.

Index	UL.	LL.	$\lambda$	$f_L$	$f_V$	$f_{LANL}$	$A_L$	$L/V$
1	$3d^2(^3F_2)$	$3d4p(^3D_1)$	113.73	6.06E-02	5.97E-02	6.45E-02	5.21E+10	1.02
2		$3d4p(^3D_2)$	113.62	1.12E-02	1.11E-02	1.27E-02	5.81E+09	1.02
3		$3d4p(^3D_3)$	113.45	3.22E-04	3.15E-04	3.19E-03	1.19E+08	1.02
4		$3d4p(^3F_2)$	113.33	3.22E-02	3.15E-02	9.88E-03	1.67E+10	1.02
5		$3d4p(^3F_3)$	113.23	4.03E-03	3.93E-03	1.65E-03	1.50E+09	1.02
6	$3d^2(^3F_3)$	$3d4f(^3G_3)$	78.74	1.14E+00	1.34E+00	7.18E-01	8.76E+11	0.85
7		$3d4f(^3D_1)$	78.48	2.56E-02	2.99E-02	1.68E-02	4.63E+10	0.86
8		$3d4f(^3D_2)$	78.49	4.75E-03	5.53E-03	5.10E-03	5.14E+09	0.86
9		$3d4f(^3D_3)$	78.5	1.36E-04	1.58E-04	2.33E-02	1.05E+08	0.86
10		$3d4p(^3D_2)$	113.85	6.43E-02	6.32E-02	5.48E-02	4.63E+10	1.02
11	$3d^2(^3F_4)$	$3d4p(^3D_3)$	113.68	8.05E-03	7.89E-03	3.75E-02	4.16E+09	1.02
12		$3d4p(^3F_2)$	113.56	2.88E-03	2.82E-03	1.71E-02	2.08E+09	1.02
13		$3d4p(^3F_3)$	113.46	3.05E-02	2.98E-02	6.13E-03	1.58E+10	1.02
14		$3d4p(^3F_4)$	113.33	2.92E-03	2.84E-03	3.42E-03	1.18E+09	1.03
15		$3d4p(^3D_3)$	113.99	7.26E-02	7.11E-02	2.97E-02	4.79E+10	1.02
16	$3d^2(^3P_0)$	$3d4p(^3F_3)$	113.77	2.27E-03	2.22E-03	5.07E-02	1.51E+09	1.02
17		$3d4p(^3F_4)$	113.63	3.41E-02	3.32E-02	3.95E-02	1.76E+10	1.03
18		$3d4f(^3G_4)$	78.95	5.54E-02	6.52E-02	7.34E-02	5.93E+10	0.85
19		$3d4f(^3G_5)$	78.9	1.08E+00	1.27E+00	7.60E-01	9.51E+11	0.85
20		$3d4f(^3D_3)$	78.76	3.05E-02	3.57E-02	2.38E-02	4.22E+10	0.85
21	$3d^2(^3P_1)$	$3d4p(^3D_1)$	117.56	2.78E-02	2.71E-02	4.43E-02	4.47E+09	1.02
22		$3d4p(^3P_1)$	116.09	8.44E-02	8.04E-02	7.22E-02	1.39E+10	1.05
23		$3d4p(^3D_1)$	117.64	6.95E-03	6.79E-03	4.08E-03	3.35E+09	1.02
24		$3d4p(^3D_2)$	117.52	2.09E-02	2.03E-02	3.13E-02	6.05E+09	1.03
25		$3d4p(^3P_1)$	116.17	2.11E-02	2.01E-02	2.61E-02	1.04E+10	1.05
26	$3d^2(^3P_2)$	$3d4p(^3P_0)$	116.32	2.81E-02	2.69E-02	3.22E-02	4.16E+10	1.05
27		$3d4p(^3P_2)$	115.86	3.53E-02	3.34E-02	3.01E-02	1.05E+10	1.06
28		$3d4p(^3P_1)$	116.31	2.11E-02	2.01E-02	1.23E-02	1.74E+10	1.05
29		$3d4p(^3P_2)$	116	6.36E-02	6.02E-02	7.29E-02	3.15E+10	1.06
30		$3d4p(^3D_2)$	117.67	4.18E-03	4.07E-03	1.85E-03	2.01E+09	1.03
31	$3d^2(^1D_2)$	$3d4p(^3D_3)$	117.49	2.34E-02	2.28E-02	9.23E-03	8.09E+09	1.03
32		$3d4p(^1D_2)$	117.47	6.48E-02	6.33E-02	3.27E-02	3.13E+10	1.02
33		$3d4p(^1F_3)$	114.8	7.58E-03	7.07E-03	5.25E-03	2.74E+09	1.07
34		$3d4p(^1P_1)$	114.18	4.00E-02	3.69E-02	2.95E-02	3.41E+10	1.08
35		$3d4f(^1P_1)$	78.6	4.35E-02	4.99E-02	2.20E-02	7.82E+10	0.87
36	$3d^2(^1G_4)$	$3d4p(^1F_3)$	116.53	1.09E-01	1.09E-01	1.22E-01	6.90E+10	1.01
37	$3d4s(^3D_1)$	$3d4p(^3P_2)$	892.33	2.59E-03	2.80E-03	5.80E-03	1.30E+07	0.93
38		$3d4p(^3P_0)$	920.16	5.02E-02	5.77E-02	8.93E-02	1.19E+09	0.87
39		$3d4p(^3P_1)$	910.84	3.81E-02	4.28E-02	1.06E-01	3.06E+08	0.89
40	$3d4s(^1D_2)$	$3d4p(^1P_1)$	887.63	9.38E-02	1.00E-01	1.57E-01	1.32E+09	0.94

**Fig. 3a.** The variation of fine structure parameter  $\zeta_2/Z$  with  $Z$ .**Fig. 3b.** The  $Z$ -dependence of the oscillator strength for the transition  $3d^2 3d4p \ ^3P_2$

For ions from nickel to zinc there are no data available at NIST online database. The present  $f$ -values of the Ni IX ion have been compared with those in reference [20] (see Table 8), the comparison shows that the ab-initio results from LANL are close to those in Ref. [20] than the data calculated by CIV3. The behavior of the oscillator strength of a given transition along an isoelectronic sequence can be illustrated using the formula [68]

$$f = f_0 + Z^{-1}f_1 + \dots \quad (6)$$

The  $Z$ -dependence of oscillator strengths may be shown in the plot of oscillator strengths for the transition  $3d^2(^3P_2)$ - $3d4p(^3P_2)$  versus the nuclear charge in figure (3b). The

present calculations decrease with increasing  $Z$ , while the  $f$ -values by NIST [67] follow non-specific behavior with  $Z$ .

Another criterion is used to determine the accuracy of oscillator strengths, the precision of the theoretical oscillator strengths can be judged by the convergence between length and velocity gauge values. If exact wave functions are used then  $f_L = f_V$  [70, 71]. For most of the present transitions the length and velocity gauge values are in a fairly good agreement, where the ratio  $L/V$  for most transitions are about one. The good agreement between  $f_L$  and  $f_V$  gives some indications (but not sufficient) for the present calculations accuracy [72].

**Table 8.** Comparison between the present calculations of oscillator strengths for Ca-like ions and those in the literature, see explanation of tables.

LL.	UL.	CIV3	LANL	NIST	Other $f$ -values
Co VIII					
$3d^2(^3F_2)$	$3d4p(^3D_2)$	1.28E-02	1.90E-02		2.14E-02 <sup>a</sup>
$3d^2(^3F_3)$	$3d4p(^3F_4)$	3.34E-03	4.05E-03	4.10E-03	4.14E-03 <sup>d</sup> , 4.10E-03 <sup>b</sup> , 4.14E-03 <sup>c</sup>
$3d^2(^3F_4)$	$3d4p(^3F_3)$	2.60E-03	3.39E-02	2.90E-02	2.89E-02 <sup>d</sup> , 2.90E-02 <sup>b</sup> , 1.01E-02 <sup>a</sup> , 2.89E-02 <sup>c</sup>
$3d^2(^3P_1)$	$3d4p(^3P_2)$	4.08E-02	4.04E-02	3.60E-02	3.67E-02 <sup>d</sup> , 3.70E-02 <sup>b</sup> , 6.87E-02 <sup>a</sup>
$3d^2(^3P_2)$	$3d4p(^3P_1)$	2.45E-02	2.07E-02	3.20E-02	3.20E-02 <sup>d</sup> , 3.20E-02 <sup>b</sup> , 3.28E-02 <sup>a</sup>
$3d^2(^3P_2)$	$3d4p(^3D_3)$	2.69E-02	2.02E-02	4.20E-02	4.20E-02 <sup>d</sup> , 4.20E-02 <sup>b</sup> , 4.32E-02 <sup>a</sup>
$3d^2(^3P_2)$	$3d4f(^3D_3)$	2.08E-01	1.51E-01	1.80E-01	1.84E-01 <sup>d</sup> , 5.90E-01 <sup>e</sup> , 1.80E-01 <sup>b</sup> , 1.24E-01 <sup>a</sup> , 1.80E-01 <sup>c</sup>
$3d^2(^1D_2)$	$3d4f(^1F_3)$	2.45E-01	2.08E-01	2.30E-01	2.34E-01 <sup>d</sup> , 5.90E-01 <sup>e</sup> , 2.80E-01 <sup>b</sup> , 1.62E-01 <sup>a</sup> , 2.20E-01 <sup>c</sup>
$3d^2(^1G_4)$	$3d4p(^1F_3)$	1.34E-01	1.50E-01	2.00E-01	1.98E-01 <sup>d</sup> , 2.00E-01 <sup>b</sup> , 2.25E-01 <sup>a</sup>
$3d^2(^1S_0)$	$3d4p(^1P_1)$	1.44E-01	1.50E-01		1.60E-01 <sup>a</sup>
Ni IX					
$3d^2(^3F_3)$	$3d4f(^3F_3)$	9.01E-02	1.31E-01		2.18E-01 <sup>a</sup>
$3d^2(^3F_4)$	$3d4f(^3F_4)$	1.01E-01	1.34E-01		2.28E-01 <sup>a</sup>
$3d^2(^3P_1)$	$3d4p(^3D_2)$	2.04E-02	3.18E-02		5.77E-02 <sup>a</sup>
$3d^2(^3P_2)$	$3d4f(^3D_3)$	2.31E-01	1.70E-01		1.51E-01 <sup>a</sup>
$3d^2(^1D_2)$	$3d4f(^1D_2)$	1.34E-01	2.26E-01		3.44E-01 <sup>a</sup>
$3d^2(^1D_2)$	$3d4f(^1F_3)$	2.70E-01	2.36E-01		1.98E-01 <sup>a</sup>
$3d^2(^1D_2)$	$3d4f(^1P_1)$	1.02E-02	2.10E-02		1.80E-02 <sup>a</sup>

Note:

a: The oscillator strengths from Ref. [20]

b: The oscillator strengths from Ref. [45]

c: The oscillator strengths from Ref. [48]

d: The oscillator strengths from Ref. [26]

e: The oscillator strengths from Ref. [44]

## 4. Conclusion

In the present study, configuration interaction calculations using CIV3 code and ab-initio calculations using the LANL code have been performed for Ca-like ions. An extensive calculations of energy levels, oscillator strengths, and radiative rates have been evaluated for configuration arrays including the  $3d^2$ ,  $3d4s$ ,  $3d4p$ ,  $3d4d$ , and  $3d4f$  levels with different angular momenta and parity. The present calculations of energies and oscillator strengths have been compared with the available experimental and theoretical sources, and it show a reasonable agreement with the literature. The atomic structure data are useful for many applications such as the identification of the solar spectra, the plasma diagnostics, and the thermonuclear fusion researches. In this paper we mentioned some data we obtained, not all the data we calculated, Such as

tables include energy levels for Ca like ions ( $Z=22-30$ ) except Fe, ions and tables include oscillator strength for Co VIII, Ni IX, Cu X, Zn XI ions, also the table includes comparison our data with the other published literature.

## References

- [1] W. Cady, Phys. Rev. 43 (1933) 322.
- [2] E. Alexander, U. Feldman, B. S. Fraenkel, S. Hoory, J. Opt. Soc. Am. 56 (1966) 651.
- [3] M. Even-Zohar, B. S. Fraenkel, J. Opt. Soc. Am. 58 (1968) 1420.
- [4] B. Warner, R. C. Krikpatrick, Mon. Not. R. Astr. Soc. 144 (1969) 397.

- [5] B. Fawcett, R. Cowan, *Solar Phys.* 31 (1973) 339.
- [6] J. Ekberg, *Phys. Scr.* 23 (1981) 7.
- [7] H. Nussbaumer, P. J. Storey, *Astron. Astrophys.* 113 (1982) 21.
- [8] E. Charro, I. Martin, *Astrophys. J.* 513 (1999) 997.
- [9] J. K. Lepson, P. Beiersdorfer, G. V. Brown, D. A. Liedah, S. B. Utter, N. S. Brickhouse, A. K. Dupree, J. S. Kaastra, R. Mewe, S. M. Kahn, *Astrophys. J.* 578 (2002) 648.
- [10] D. C. Morton, *Astrophys. J. Suppl. Ser.* 149 (2003) 205.
- [11] E. Tr`abert, A. G. Calamai, G. Gwinner, E. J. Knystautas, E. H. Pinnington, A. Wolf, *J. Phys. B* 36 (2003) 1129.
- [12] G. Y. Liang, T. M. Baumann, J. R. C. Lopez-Urrutia, S. W. Epp, H. Tawara, A. Gonchar, P. H. Mokler, G. Zhao, J. Ullrich, *Astrophys. J.* 696 (2009) 2275.
- [13] P. R. Young, K. A. Berrington, A. Lobel, *Astron. Astrophys.* 432 (2005) 665.
- [14] J. Zeng, G. Y. Liang, G. Zhao, J. R. Shi, *Mon. Not. R. Astron. Soc.* 357 (2005) 440.
- [15] T. Holczer, E. Behar, S. Kaspi, *Astrophys. J.* 632 (2005) 788.
- [16] P. R. Young, E. Landi, *Astrophys. J.* 707 (2009) 173.
- [17] G. D. Zanna, *Astron. Astrophys.* 508 (2009) 501.
- [18] G. D. Zanna, *Astron. Astrophys.* 537 (2012) A38(17pp).
- [19] M. C. Witthoeft, N. R. Badnell, *Astron. Astrophys.* 481 (2008) 543.
- [20] P. Quinet, J. E. Hansen, *J. Phys. B* 29 (1996) 1879.
- [21] J. R. Roberts, T. Andersen, G. Sorensen, *Astrophys. J.* 181 (1973) 567.
- [22] Y. Baudinet-Robinet, P. D. Dumont, H. P. Garnir, N. Grevesse, E. Biemont, *J. Opt. Soc. Am.* 70 (1980) 464.
- [23] D. C. Abbott, *J. Phys. B* 11 (1973) 3479.
- [24] S. Kastner, *Solar Phys.* 151 (1994) 41.
- [25] J. Ekberg, U. Feldman, *Astrophys. J. Suppl. Ser.* 148 (2003) 567.
- [26] B. Fawcett, A. Ridgeley, J. Ekberg, *Phys. Scr.* 21 (1980) 155.
- [27] A. Raassen, P. Uylings, *Astron. Astrophys. Suppl. Ser.* 123 (1997) 147.
- [28] U. I. Safronova, W. R. Johnson, D. Kato, S. Ohtani, *Phys. Rev. A* 63 (2001) 032518 (11pp).
- [29] U. I. Safronova, A. S. Safronova, *J. Phys. B* 43 (2010) 074026 (15pp).
- [30] R. Faulkner, M. Wang, P. Dunne, A. Arnesen, F. Heijkenskj, R. Hallin, G. O'Sullivan, *J. Phys. B* 34 (2001) 593.
- [31] E. Biemont, J. E. Hansent, P. Quinets, C. J. Zeippen, *J. Phys. B* 25 (1992) 5029.
- [32] S. Haq, R. Ali, M. Kalyar, M. Raq, A. Nadeem, M. Baig, *Eur. Phys. J. D* 50 (2008) 1.
- [33] A. N. Ryabtsev, E. Y. Kononov, S. S. Churilov, *Opt. Spectrosc.* 106 (2009) 163.
- [34] T.-Y. Zhang, N.-W. Zheng, D.-X. Ma, *Int. J. Quant. Chem.* 109 (2009) 145.
- [35] A. El-maaref, Z. Samak, S. Allam, T. El-Sherbini, *Int. J. New. Hor. Phys.* 2 (2015) 25.
- [36] M. Grieve, C. Ramsbottom, *Mon. Not. R. Astron. Soc.* 424 (2012) 2461.
- [37] W. L. Wiese, M. W. Smith, B. M. Miles, *Tech. rep., National Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.)* (1969).
- [38] M. W. Smith, W. L. Wiese, *J. Phys. Chem. Ref. Data* 2 (1973) 85.
- [39] D. C. Morton, *Astrophys. J. Suppl. Ser.* 77 (1991) 119.
- [40] C. Corliss, J. Sugar, *J. Phys. Chem. Ref. Data* 8 (1979) 1.
- [41] J. Sugar, C. Corliss, *J. Phys. Chem. Ref. Data* 14 Supplement 2 (1985) 1.
- [42] J. Sugar, A. Musgrove, *J. Phys. Chem. Ref. Data* 19 (1990) 527.
- [43] J. Sugar, A. Musgrove, *J. Phys. Chem. Ref. Data* 24 (1995) 1803.
- [44] J. R. Fuhr, G. A. Martin, W. L. Wiese, S. M. Younger, *J. Phys. Chem. Ref. Data* 10 (1981) 305.
- [45] J. Fuhr, G. Martin, W. Wiese, *J. Phys. Chem. Ref. Data* 17 Supplement 4 (1988) 1.
- [46] G. Martin, W. Fuhr, W. Wiese, *J. Phys. Chem. Ref. Data* 17 Supplement 3 (1988) 1.
- [47] V. Kaufman, J. Sugar, *J. Phys. Chem. Ref. Data* 17 (1988) 1679.
- [48] T. Shirai, A. Mengoni, Y. Nakai, J. Sugar, W. L. Wiese, K. Mori, H. Sakai, *J. Phys. Chem. Ref. Data* 21 (1992) 23.
- [49] T. Shirai, Y. Nakai, T. Nakagaki, J. Sugar, W. L. Wiese, *J. Phys. Chem. Ref. Data* 22 (1993) 1279.
- [50] T. Shirai, J. Sugar, A. Musgrove, W. L. Wiese, *J. Phys. Chem. Ref. Data Monograph* 8 (2000) 1.
- [51] T. Shirai et al., *At. Data Nucl. Data Tables* 37 (1987) 235.
- [52] A. Hibbert, *Comput. Phys. Commun.* 9 (1975) 141.
- [53] R. Glass, A. Hibbert, *Comput. Phys. Commun.* 16 (1978) 19.
- [54] M. Mohan, A. Hibbert, *Phys. Scr.* 44 (1991) 158.
- [55] A. Hibbert, M. Le Dourneuf, M. Mohan, *At. Data Nucl. Data Tables* 53 (1993) 23.
- [56] H. M. S. Blackford, A. Hibbert, *At. Data Nucl. Data Tables* 58 (1994) 101.
- [57] D. McPeake, A. Hibbert, *J. Phys. B* 33 (2000) 2809.
- [58] A. A. El-Maaref, M. A. M. Uosif, S. H. Allam, Th. M. El-Sherbini, *At. Data Nucl. Data Tables* 98 (2012) 589.
- [59] A. A. El-Maaref, S. H. Allam, Th. M. El-Sherbini, *At. Data Nucl. Data Tables* 100 (2014) 155.

- [60] A. A. El-Maaref, M. Ahmad, S. H. Allam, At. Data Nucl. Data Tables 100 (2014) 781.
- [61] M. P. Donnelly, A. Hibbert, Mon. Not. R. Astron. Soc. 302 (1999) 413.
- [62] P. Oliver, A. Hibbert, J. Phys. B 40 (2007) 2847.
- [63] E. Clementi, C. Roetti, At. Data Nucl. Data Tables 14 (1974) 177.
- [64] R. D. Cowan, The Theory of Atomic Structure and Spectra; University of California Press: Berkeley, CA, USA, 1981.
- [65] Th. M. El Sherbini, Z. Physik A 275 (1975) 1.
- [66] Th. M. El Sherbini, A. A. Farrag, J. Phys. B 9 (1976) 2797.
- [67] NIST Atomic Spectra Database: <http://www.nist.gov/pml/data/asd.cfm>.
- [68] A. Hibbert, Rep. Progr. Phys. 38 (1975) 1217.
- [69] A. Hibbert, Phys. Scr. T65 (1996) 104.
- [70] A. A. El-Maaref, S. Schippers, A. Muller, Atoms 3 (2015) 2.
- [71] J. A. Tully, M. J. Seaton, K. A. Berrington, J. Phys. IV 1 (1991) C1: 169.
- [72] A. A. El-Maaref, J. Quant. Spectrosc. Radiat. Transf. (2016) 45.