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Experimental and Theoretical Study of the $5s^25p^3$ and $5s5p^4$ Configurations in Sb-like Cerium

Research Article

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Abstract. In this paper the ground and first excited configurations of Ce VIII have been studied, both experimentally and theoretically. The spectra of cerium have been photographed using a spark source on a normal incident spectrograph, equipped with a grating having the reciprocal dispersion of 1.38 Å/mm in the first order. The ground configuration has been established experimentally for the first time. The GRASP2018 package has been used to calculate energy levels, wavelengths and transition rates for the $5s^25p^3$ and $5s5p^4$ configurations. The electron correlation effects, Breit interaction and quantum electrodynamics effects have been considered in the calculation. The experimentally established energy levels have been compared with their theoretical values.

Keywords. Energy levels; Transition rates; Lifetime; Cowan's code; GRASP2018

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1. Introduction

Spectroscopic studies of rare earth elements are important for astrophysics and plasma science. Kinetics modelling of the laboratory as well as astrophysical plasma requires accurate radiative transition rates [1]. Also, highly charged ions are proposed for creation of ultra-accurate atomic clocks [2]. All these applications require accurate data on multi-charged Ce ions.

Seven times ionized cerium (Ce VIII) is a member of Sb I isoelectronic series. It has $5s^25p^3$asthe ground configuration. Excitation from the outer $n = 5$ shells leads to the configurations of the type $5s5p^4$and $5s^25p^2nl$. Excitation from $4d^{10}$ core leads to the $4d^95s^25p^3nl$

configurations. An analysis of this spectrum along with Ce VII was done by Tauheed et al. [3], where only three excited levels, namely, $^4P_{5/2}$, $^4P_{3/2}$ and $^4P_{1/2}$ of the $5s5p^4$ configuration have been reported. Recently, Gaynor et al. [4] employed the dual laser-produced plasma technique to study the $4d^95s^25p^4$ core-excited configuration of Ce VIII.

In the present work, the spectra of cerium have been recorded using a normal incidence grating spectrograph. The study began with the calculations using Cowan's code [5] for the $5s^25p^3$-$5s5p^4$ transition array. To verify our analysis, we have performed independent calculations for the ground and first excited configurations of Ce VIII using the GRASP2018 package. It is based on fully relativistic multi-configuration Dirac-Hartree-Fock (MCDHF) wave functions [6]. Theoretical energy levels, oscillator strength and transition rates have been calculated. The experimentally observed levels have been compared with the calculated levels by the GRASP2018 package.

2. Experimental Details

The spectra used in the present work were recorded at St. Fransis Xavier University, Antigonish, Canada. It was recorded on Kodak SWR plates using 3 m normal incidence vacuum spectrograph under varied experimental conditions such as changing the charging potential and varying the circuit inductance. The spectrograph setup is equipped with 2400 lines per mm, holographic grating with a resolution of 1.38 Å/mm in the first order along with triggered spark source. The source circuit consists of a 14.5 μF low-inductance fast charging capacitor and a trigger module that could generate pulses up to 30 kV to initiate the spark discharge. The recorded spectrum was measured using Zeiss Abbe comparator at Aligarh Muslim University, Aligarh. The intensities were visually estimated based on human eye from the blackening of the photographic plates. The wavelengths have calibrated using the internal standard of carbon, oxygen [7] and Ce V [8] lines by a computer program MOSFIT [9], which does polynomial fits with various degrees of freedom.

3. Calculations

Relativistic calculations were performed using the GRASP2018 package [6]. Further details of the package can be found elsewhere [10]. Ce VIII calculations have been done parity-wise i.e., even and odd states were determined separately in the extended optimization level (EOL) scheme. Energy levels, oscillator strength and transition rates have been calculated taking Breit interaction (BI) and quantum electrodynamic (QED) effects into account through large CSFs expansions for $n = 8$ complex for $5s^25p^3$, $5s5p^4$, $5s^25p^25d$ and $5s^25p^26s$ configurations. The convergence of the energy levels is obtained with the increase of the active set. The valance (V) and core-valance (CV) electron correlation effects are accounted for expansions obtained from CSFs through single-double multireference (SD-MR) expansions to increase active sets of orbitals [11, 12]. The agreement between transition rates computed in length and velocity form reflects the accuracy of our results. The relative difference can be used as an indicator of uncertainty dT [13, 14].

$$dT = \frac{|A_l - A_v|}{\max(A_l, A_v)}.$$

4. Analysis and Results

The cerium spectra have been recorded on 3-m normal incidence spectrograph in the 300-1200 Å region. Ce VIII lines appear on our plates with reasonably good intensity. We have confirmed and extended the earlier reported workby Tauheed and Joshi [3].

The resonance transition array $5s^25p^3$-$5s^1p^4$ in Ce VIII produces dozens of lines. For the prediction of these lines, $5s^25p^3$-$5s^1p^4$ transitions have been calculated with inclusion of the $5s^25p^25d$ and $5s^25p^26s$ configurations by Cowan's computer code [5]. The Slater parameters were scaled as 100% of the HF values for the E_{av} and ζ_{nl} parameters, 85% for F^k, 75% for G^k and, 80 % for CI parameters. The predicted lines produced by the Cowan code have been identified in the recorded spectrum with the help of Find3 [15] program and classified in $5s^25p^3$-$5s5p^4$ transitions array. The identified transitions are fed into the input of the computer code LOPT [16]. It drives energy level values, optimized from the observed transition wavelengths. It also calculates the uncertainties of the levels and estimate Ritz wavelength of classified transitions. We have established all the ground state energy levels of Ce VIII for the first time. The work has been extended to establish 4 new levels of $5s5p^4$ configuration. All the experimentally established energy levels (E_{obs}) along with percentage composition in LS coupling scheme are given in Table 1. The observed energy levels have been compared with independently calculated energy levels using GRASP2018 code. E_{obs} and E_{cal} are seemed to be in good agreement as depicted in Table 1.

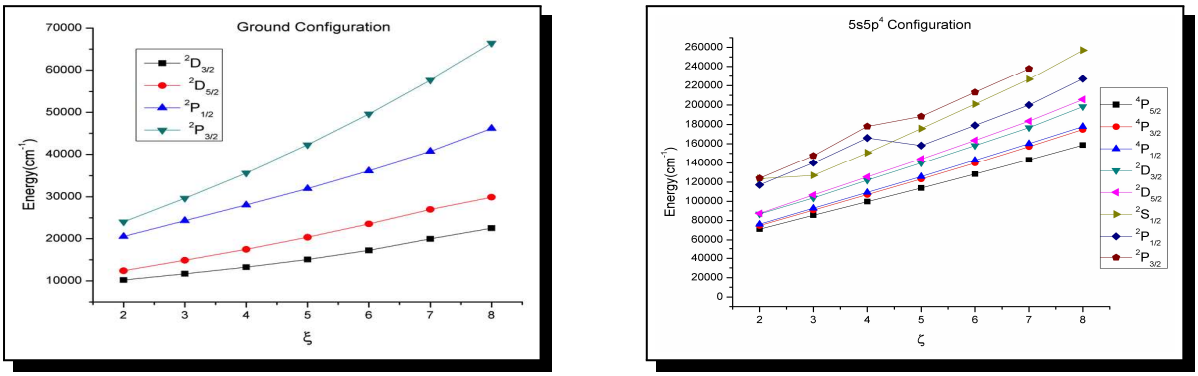
Table 1. Observed (E_{obs}) and calculated (E_{cal}) energy levels with eigenvector composition in cm^{-1}

State	LS-composition	E_{obs}.(cm^{-1})	E_{cal}.(cm^{-1})	Diff.[a]
$5p^3$ $^4S_{3/2}$	63% + 23% $5p^3$ ^2P + 11% $5p^3$ ^2D	0	0	-
$5p^3$ $^2D_{3/2}$	60% + 20% $5p^3$ ^4S + 8% $5p^3$ ^2P	22528.7	22768	1.06
$5p^3$ $^2D_{5/2}$	93%	29878.0	30664	2.63
$5p^3$ $^2P_{1/2}$	94%	46180.9	46687	0.01
$5p^3$ $^2P_{3/2}$	63% + 21% $5p^3$ ^2D + 8% $5p^3$ ^4S	66418.1	66552	0.20
$5s5p^4$ $^4P_{5/2}$	82% + 7% $5s5p^4$ ^2D + 7% $5s5p^4$ ^4P	158620.3[T]	157969	0.40
$5s5p^4$ $^4P_{3/2}$	79% + 07% $5s5p^4$ ^4P + 6% $5s5p^4$ ^2D	174758.3[T]	174222	0.30
$5s5p^4$ $^4P_{1/2}$	76% + 12% $5s5p^4$ ^2S + 7% $5s5p^4$ ^4P	177774.0	177752	0.01
$5s5p^4$ $^2D_{3/2}$	60% + 11% $5s5p^4$ ^2D + 9% $5s5p^4$ ^4P	198225.2	198463	0.12
$5s5p^4$ $^2D_{5/2}$	69% + 13% $5s5p^4$ ^2D + 7% $5s5p^4$ ^4P	205582.9	205255	0.16
$5s5p^4$ $^2S_{1/2}$	33% + 27% $5s5p^4$ ^2P + 17% $5p^25d$ ^2P	226958.3	227401	0.19
$5s5p^4$ $^2P_{3/2}$	25% + 24% $5p^25d$ ^4F + 21% $5p^25d$ ^2P		228694	
$5s5p^4$ $^2P_{1/2}$	20% + 20% $5s5p^4$ ^2S + 18% $5p^25d$ ^2P	256978.2	257793	0.30

[a] The absolute % difference between the optimized(experimental) and GRASP2018(calculated) level values, $\% \, diff. = \left|\frac{E_{obs}-E_{Cal}}{E_{obs}}\right| \times 100$

[T]Levels established by Tauheed and Joshi [3]

The ground configuration $5s^25p^3$ consist of 5 levels $^2D_{3/2}$, $^2D_{5/2}$, $^2P_{1/2}$, $^2P_{3/2}$ and $^4S_{3/2}$. Ce VIII was analyzed for the first time by Tauheed et al. in 2008. They established three levels of $5s5p^4$ configuration using single transition connected with the ground most level $^4S_{3/2}$ at 0.0 cm^{-1}. Fortunately, we have get three additional transitions for $^4P_{5/2}$ and also, three additional transitions for $^4P_{3/2}$, which confirms both the earlier reported levels. But for $^4P_{1/2}$, reported earlier at 177988.8 cm^{-1} no additional transitions could be found, instead a new level value at 177774.0 cm^{-1}has been observed with 3 supportive transitions. Further this level is following the trend exhibited by the iso electronic plot for Sb-I sequence as shown in Figure 1 [17–24]. Hence we propose 177774.0 cm^{-1} as $^4P_{1/2}$ level.



(a) **(b)**

Figure 1. (a) Isoelectronic plot of the energy levels of ground configuration and (b) Isoelectronic plot of $5s5p^4$ configuration. E is the energy of the level in cm^{-1} and ξ is the charge number of the ion ($\xi = 8$ for Ce VIII)

Except $^4S_{3/2}$, all the other four levels of ground configuration were still unknown. During our analysis, ^4P levels of 5s5p4 helped us to establish these four levels of ground configuration for the first time. Each level has 5 to 6 supporting transitions except the $^2P_{1/2}$ that has been establish by three supporting transitions. Once all the ground levels were established, we have also got doublets ($^2D_{3/2}$, $^2D_{5/2}$, $^2S_{1/2}$ and $^2P_{1/2}$) of $5s5p^4$ configuration. But the $^2P_{3/2}$ of this configuration could not be established because of strong mixing with ^4F and ^2P of $5p^35d$. The observed $5s^25p^3$-$5s^1p^4$ transitions are shown in Table 2 with their calculated transition probabilities, oscillator strength and Ritz wavelengths.

Table 2. Classified lines of Ce VIII along with their wavelengths (Å), transition probabilities (s^{-1}) and weighted oscillator strength

Lower	J	Upper	J	I^c_{obs}	λ_{obs}	λ_{Ritz}	dw^d_{O-C}	Tra. Prob.^{e}	$g_{low}f$ ^{e}	dT
$5p^3\ ^2D$	3/2	$5s5p^4\ ^2P$	1/2	85	426.529	426.531	0.012	1.28E+09	7.04E-02	0.097
$5p^3\ ^4S$	3/2	$5s5p^4\ ^2S$	1/2	88	440.622	440.6096	0.014	9.95E+08	5.80E-02	0.143
$5p^3\ ^4S$	3/2	$5s5p^4\ ^2D$	5/2	75	486.422	486.422	-0.001	1.66E+07	3.53E-03	0.480
$5p^3\ ^2D$	3/2	$5s5p^4\ ^2S$	1/2	77	489.149	489.166	-0.011	3.89E+09	2.80E-01	0.075
$5p^3\ ^4S$	3/2	$5s5p^4\ ^2D$	3/2	74	504.486	504.477	0.010	3.38E+08	5.18E-02	0.040
$5p^3\ ^2D$	3/2	$5s5p^4\ ^2D$	5/2	53	546.29	546.286	0.007	7.23E+06	1.97E-03	0.369
$5p^3\ ^2P$	1/2	$5s5p^4\ ^2S$	1/2	66	553.176	553.166	0.014	1.85E+09	1.72E-01	0.217
$5p^3\ ^4S$	3/2	$5s5p^4\ ^4P$	1/2	70	562.502	562.512	-0.013	1.66E+09	1.59E-01	0.019
$5p^3\ ^2D$	5/2	$5s5p^4\ ^2D$	5/2	75^B	569.147	569.136	0.012	1.73E+09	5.14E-01	0.005
$5p^3\ ^2D$	3/2	$5s5p^4\ ^2D$	3/2	75^B	569.147	569.163	-0.010	2.48E+09	4.84E-01	0.005
$5p^3\ ^4S$	3/2	$5s5p^4\ ^4P$	3/2	65	572.185*	572.183	-0.002	1.62E+09	3.20E-01	0.010
$5p^3\ ^2P$	3/2	$5s5p^4\ ^2S$	1/2	73	622.891	622.897	-0.003	1.97E+07	2.29E-03	0.328
$5p^3\ ^4S$	3/2	$5s5p^4\ ^4P$	5/2	64	630.437*	630.436	-0.002	7.70E+08	2.79E-01	0.033
$5p^3\ ^2D$	3/2	$5s5p^4\ ^4P$	1/2	86	644.147	644.142	0.008	8.44E+07	1.06E-02	0.084
$5p^3\ ^2D$	3/2	$5s5p^4\ ^4P$	3/2	87^w	656.876	656.902	-0.023	3.79E+05	9.97E-05	0.525
$5p^3\ ^2D$	5/2	$5s5p^4\ ^4P$	3/2	60	690.223	690.225	-0.002	6.49E+07	1.90E-02	0.136
$5p^3\ ^2P$	3/2	$5s5p^4\ ^2D$	5/2	75	718.569	718.573	-0.007	3.83E+08	1.81E-01	0.153
$5p^3\ ^2D$	3/2	$5s5p^4\ ^4P$	5/2	84	734.807	734.799	0.015	2.21E+08	1.09E-01	0.007
$5p^3\ ^2P$	3/2	$5s5p^4\ ^2D$	3/2	65	758.682	758.684	-0.001	4.92E+06	1.71E-03	0.683
$5p^3\ ^2P$	1/2	$5s5p^4\ ^4P$	1/2	56	759.92	759.918	0.001	1.19E+08	2.10E-02	0.099
$5p^3\ ^2D$	5/2	$5s5p^4\ ^4P$	5/2	62	776.746	776.745	0.004	8.93E+07	4.99E-02	0.010
$5p^3\ ^2P$	1/2	$5s5p^4\ ^4P$	3/2	30	777.735	777.742	-0.008	1.55E+06	5.80E-04	0.477
$5p^3\ ^2P$	3/2	$5s5p^4\ ^4P$	3/2	81^w	923.047	923.018	0.019	2.80E+07	1.46E-02	0.700
$5p^3\ ^2P$	3/2	$5s5p^4\ ^4P$	5/2	60	1084.569	1084.573	-0.009	2.41E+06	2.62E-03	0.360

^{c} Relative intensities (see in text)
^{w} wide
^{B} blended, ^{c} Calculated by GRASP2018, (g_{low} statistical weight of lower level)
* Classified by Tauheed and Joshi [3]

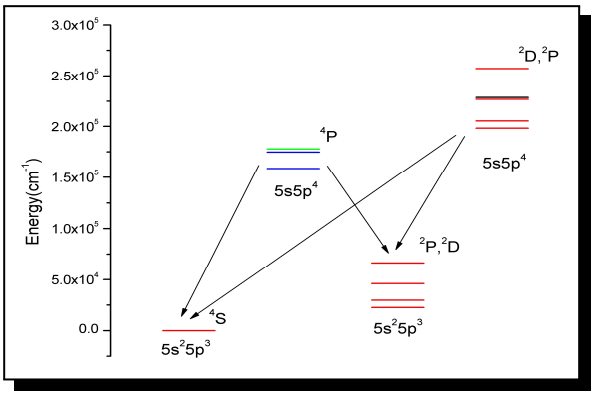


Figure 2. $5s^25p^3$ and $5s5p^4$ levels. Energy levels shown in blue are from [3], and those shown in red are newly established. The revised level is shown in green and the predicted one is in black

5. Summary and Conclusions

The study of seven times ionized cerium has been carried out experimentally as well as theoretically for the $5s^25p^3$-$5s5p^4$transition array. The spectra have been recorded on 3m normal incidence grating spectrograph. All the energy levels of ground configuration have been established for the first time. For the excited $5s5p^4$ configuration out of 7 only 3 were reported earlier, of which two $^4P_{5/2}$ and $^4P_{3/2}$ has been confirmed with six extra supportive transitions, however $^4P_{1/2}$ has been revised, and remaining 4 levels have also been established. The isoelectronic trend also supports the experimental levels.

Theoretical calculations for these configurations have been performed independently using GRASP2018 package based on fully relativistic MCDHF model. Energy levels, wavelengths, transition rates and lifetimes have been obtained theoretically. The calculated energy levels are in good agreement with the experimentally observed ones.

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Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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