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Energy Levels and Transition Parameters in Ce^{6+} from MCDHF Model

Research Article

Abdul Wajid*, and S. Jabeen

Department of Physics, Aligarh Muslim University, Aligarh 202 002, India
***Corresponding author:** abdulwajidansari@live.com

Abstract. *Multiconfiguration Dirac-Hartree-Fock* (MCDHF) calculations and subsequent *Relativistic Configuration Interaction* (RCI) calculations have been performed for the $5s^25p^4$, $5s^25p^36s$ and $5s5p^5$ configurations of six times ionized cerium using GRASP2018 package. The electron correlation effects, (BI) interaction and *Quantum Electrodynamics* (QED) effects have been considered in the calculation. Energy levels, oscillator strength and transition probabilities among the transitions of $5s^25p^4$, $5s5p^5$ and $5s^25p^36s$ have been calculated. The calculated energy levels are compared with experimental data available and show good agreement with it.

Keywords. Dirac-Hartree-Fock; Energy levels; Transition probabilities; Lifetimes

PACS. 32.30.-r; 33.20.Ni; 34.80.Dp; 31.15.Ne

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1. Introduction

The spectroscopic data of atoms/ions data are required in astrophysics applications and plasma science. Also, atomic spectroscopy data is use as an input to other fields such as medical science and industrial research [1]. So far, experimental data is not fully available because of technical constraints. On the other hand with the advancement of computer technology, theoretical model are able to generate accurate data close to experimental observations. This data may be use to predict accurate observations, or direct input for other fields as well [2].

Cerium is the most abundant element on earth crust in the lanthanide group [3]. Also, the effect of cerium in the theoretical kilonova model radiation spectrum shows its formation

sign in star merger [4]. Neutral and moderately charged Cerium has been studied by many spectroscopist, but there is limited data available for cerium ions [5]. In this work, our target is to study Ce VII transitions. Tauheed et al. have reported the Ce VII transitions and the levels using vacuum spectrograph [6]. The highly charged ions are important in astrophysical plasma modeling and applications [7].

In this paper we are presenting calculated energy levels, transition parameters with fully relativistic MCDHF approach for $5s^25p^4$, $5s5p^5$ and $5s^2p^36s$ configurations of Ce VII. The earlier reported levels have been optimized to estimate the Ritz wavelengths and uncertainties using a program LOPT [8].

We have used GRASP2018 code based on *Multiconfiguration Dirac-Fock* (MCDHF) calculations and *Relativistic Configuration Interaction* (RCI) calculations [9]. It gave the opportunity,first time to present the relativistic calculations for Energy levels, oscillator and transition probabilities for Electric-dipole (E1) among the states of the ground $5s^25p^4$, and excited, $5s^2p^36s$ and $5sp^5$ configurations for six times ionized cerium. The electron correlation effects, Breit interaction and quantum electrodynamics effects have been considered in the calculation. The calculated levels are compared with the optimized experimental results and found good agreement with it. These comparisons of energy levels ensure the accuracy of chosen wave functions.

2. Theoretical Calculations

The relativistic calculations were performed using GRASP2018 package based on *Multiconfiguration Dirac-Hartree-Fock method* (MCDHF) [10, 12].

2.1 Fully Relativistic MCDHF Calculations

According to quantum mechanics Dirac-Coulomb Hamiltonian explained as

$$H_{DC} = \sum_{i=1}^{N}(c\boldsymbol{\alpha}_i + (\boldsymbol{\beta}_i - 1)c^2 + V(r_i)) + \sum_{i>j}^{N}\frac{1}{r_{ij}},$$

where $\boldsymbol{\alpha}_i$ and $\boldsymbol{\beta}_i$ are 4×4 Dirac matrices, V is the monopole part of electron-nucleus Coulomb interaction, and in MCDHF formulism the trial atomic state function ψ for a state labeled ΓPJM constitute the linear combination of configuration state function (CSF)$\phi(\gamma_r$PJM) represented as

$$\psi(\Gamma\text{PJM}) = \sum_r C_r\phi(\gamma_r\text{PJM}),$$

where C_r is the configuration mixing coefficients, P, J and M are the parity, total angular momentum and magnetic quantum numbers, respectively. CSFs are the linear combination of Slater determinant constructed from relativistic orbitals [10, 11]. The agreement between transition rates computed in length (Babushkin) and velocity (Coulomb) form reflects the accuracy of our results. The relative difference can be used as an indicator of uncertainty

dT [13, 14].

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

The calculations were made by parity, meaning that the even and odd states were determined in separate calculations in EOL scheme. The calculations of even states were based on the CFS expansion formed by $5s^2 5p^4$ configuration and of odd stated from $5s5p^5$ configuration, that define the *multi-reference* (MR) for even and odd states. Energy levels, oscillator strength and transition probabilities for electric-dipole (E1) have been calculated through large configuration state function expansions for $n = 8$ complex within the framework of *Multi-Configuration Dirac-Fock method* (MCDHF). The transverse photon interaction in the low frequency limit, vacuum polarization and self energy corrections considered in the calculation. The *valance* (V) and *core valance* (CV) electron correlation effects are accounted for expansions obtained from CSFs through *single-double multi-reference* (SD-MR) expansions to increase active sets of orbitals [10, 14].

3. Results and Discussion

Transitions of first excited even configurations in Ce VII lie in vacuum ultraviolet region. Tauheed et al. [6] reported all the energy levels of first excited $5s5p^5$ and $5s^2 5p^3 6s$ configurations along with one level of $5s^2 5p^3 5d$ configuration. Using these reported transitions we also have optimize the observed energy levels and estimate the Ritz wavelengths using a computer program LOPT. The uncertainties in wavelengths are the square root of the sum of the squares of the level uncertainties [8]. In the MCDHF calculations, the CSFs are obtained with the MR set of $5s^2 5p^4$ configuration state in even parity system and, $5s5p^5$, $5s^2 5p^3 5d$, $5s5p^4 4f$, $5s^2 5p^3 6s$ and $5s^2 5p^2 5d4f$ configuration state in odd parity system. The active set is increase in step of orbital layers and the configuration expansions then obtained by SD substitutions from the MR set to active set of orbitals for principal quantum number up to $n = 8$ for orbital angular momenta upto $l = 3$ and, $n = 5$ for $4 \le l \le 6$. The *core valance* (CV) and *valence valance* (VV) effects are taken into account for 4f, 5p, 5d and 6s while keeping the core ($1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10}$) frozen. BI and QED effects have also been considered in the RCI calculations. In all tables the quantum states are labeled with the leading term of LSJ-percentage composition. The energy levels of Ce VII, labeled in LS-coupling scheme for $5s^2 5p^4$, $5s5p^5$ and $5s^2 5p^3 6s$ configurations based on the largest orbital set $n = 8$, are presented in Table 1, together with observed energies for $5s^2 5p^4$, $5s5p^5$ and $5s^2 5p^3 6s$ configurations by Tauheed et al. [6]. In Figure 1, the differences between calculated and observed energies are shown and the agreement between calculated and observed energies is found worth. In Table 2, we give the Ritz wavelength, oscillator strengths and transition probabilities for Ce VII transitions for the first time. These lines appear in the UV spectral region from 262 to 767 Å. The average value of uncertainty indicator (dT) for these transitions found to be 0.044, which reflect the quality of chosen wave functions.

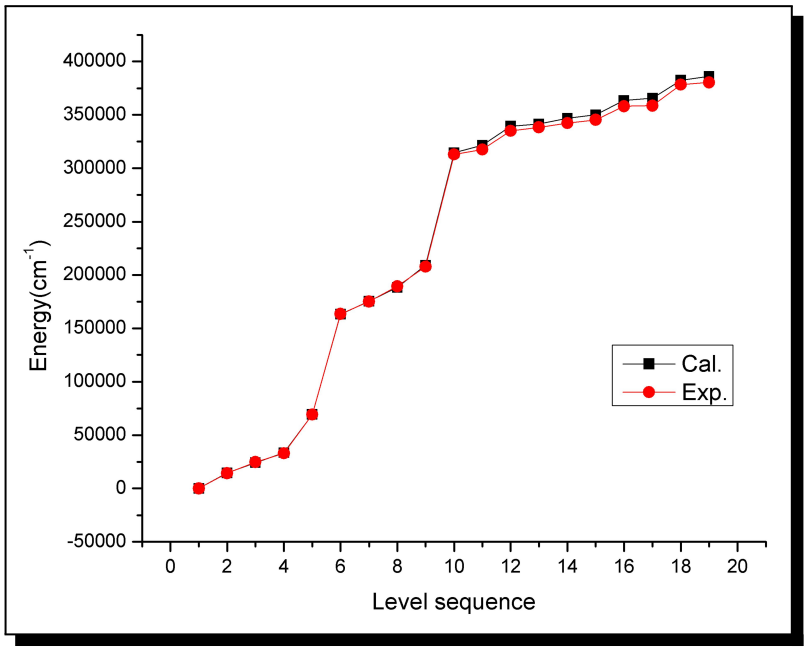

Figure 1

Table 1. Comparison between the calculated and available experimental energy levels in Ce VII

No.	State	$E_{cal.}$(cm^{-1})	$E_{exp.}$ (cm^{-1})
1	$5s^25p^4\ ^3P_2$	0	0.0
2	$5s^25p^4\ ^3P_0$	14591	14210.0
3	$5s^25p^4\ ^3P_1$	24090	24709.0
4	$5s^25p^4\ ^1D_2$	33620	33138.0
5	$5s^25p^4\ ^1S_0$	69400	69293.0
6	$5s5p^5\ ^3P_2$	163370	163427.0
7	$5s5p^5\ ^3P_1$	175318	175059.0
8	$5s5p^5\ ^3P_0$	188519	189567.0
9	$5s5p^5\ ^1P_1$	209288	207828.0
10	$5s^25p^36s\ ^5S_2$	314388	313029.0
11	$5s^25p^36s\ ^3S_1$	321419	317472.0
12	$5s^25p^36s\ ^3D_2$	339491	334936.0
13	$5s^25p^36s\ ^3D_1$	341502	338240.0
14	$5s^25p^36s\ ^3D_3$	347020	342321.0
15	$5s^25p^36s\ ^1D_2$	349908	345237.0
16	$5s^25p^36s\ ^3P_0$	363629	358164.0
17	$5s^25p^36s\ ^3P_1$	365494	358691.0
18	$5s^25p^36s\ ^3P_2$	382332	378418.0
19	$5s^25p^36s\ ^1P_1$	386006	380313.0

Table 2. Classified lines, Ritz wavelength and calculated transition parameters

I^*_{obs}	λ^*_{obs}(Å)	λ_{RITZ}(Å)	Unc.	Lower	Upper	$A(s^{-1})$	$g_{low}f$	dT
14	262.945	262.9413	0.004	$5s^25p^4\ ^3P_2$	$5p^36s\ ^1P_1$	1.16E+08	3.49E-03	0.049
12	273.144	273.1470	-0.003	$5s^25p^4\ ^3P_0$	$5p^36s\ ^1P_1$	1.21E+08	3.96E-03	0.013
10	281.211	281.2110	0.000	$5s^25p^4\ ^3P_1$	$5p^36s\ ^1P_1$	4.61E+08	1.58E-02	0.043
17	282.720	282.7180	0.002	$5s^25p^4\ ^3P_1$	$5p^36s\ ^3P_2$	1.35E+09	7.86E-02	0.039
14	288.039	288.0390	0.000	$5s^25p^4\ ^1D_2$	$5p^36s\ ^1P_1$	5.73E+09	2.08E-01	0.004
21	289.619	289.6210	-0.002	$5s^25p^4\ ^1D_2$	$5p^36s\ ^3P_2$	1.77E+09	1.08E-01	0.001
25	289.655	289.6560	-0.001	$5s^25p^4\ ^3P_2$	$5p^36s\ ^1D_2$	2.17E+09	1.34E-01	0.084
31	290.291	290.2920	-0.001	$5s^25p^4\ ^3P_0$	$5p^36s\ ^3P_1$	4.60E+09	1.68E-01	0.009
300	292.123	292.1230	0.000	$5s^25p^4\ ^3P_2$	$5p^36s\ ^3D_3$	5.48E+09	4.78E-01	0.020
37	295.643	295.6489	-0.006	$5s^25p^4\ ^3P_2$	$5p^36s\ ^3D_1$	2.68E+09	1.03E-01	0.004
81	298.564	298.5650	-0.001	$5s^25p^4\ ^3P_2$	$5p^36s\ ^3D_2$	3.54E+09	3.00E-01	0.029
19	299.416	299.4160	0.000	$5s^25p^4\ ^3P_1$	$5p^36s\ ^3P_1$	1.25E+09	4.18E-02	0.042
20	299.891	299.8910	0.000	$5s^25p^4\ ^3P_1$	$5p^36s\ ^3P_0$	5.31E+09	6.91E-02	0.015
15	307.170	307.1700	0.000	$5s^25p^4\ ^1D_2$	$5p^36s\ ^3P_1$	4.29E+09	1.75E-01	0.023
47	308.620	308.6140	0.006	$5s^25p^4\ ^3P_0$	$5p^36s\ ^3D_1$	2.88E+08	1.21E-02	0.040
65	311.984	311.9840	0.000	$5s^25p^4\ ^3P_1$	$5p^36s\ ^1D_2$	2.32E+09	1.64E-01	0.041
300	314.984	314.9880	-0.004	$5s^25p^4\ ^3P_2$	$5p^36s\ ^3S_1$	1.76E+10	7.65E-01	0.025
400	318.946	318.9470	-0.001	$5s^25p^4\ ^3P_1$	$5p^36s\ ^3D_1$	1.49E+10	6.63E-01	0.031
150	319.459	319.4590	0.000	$5s^25p^4\ ^3P_2$	$5p^36s\ ^5S_2$	2.55E+08	1.94E-02	0.050
500	320.412	320.4110	0.001	$5s^25p^4\ ^1D_2$	$5p^36s\ ^1D_2$	2.20E+10	1.65E+00	0.032
64	322.340	322.3440	-0.004	$5s^25p^4\ ^3P_1$	$5p^36s\ ^3D_2$	7.75E+08	5.84E-02	0.014
63	323.433	323.4330	0.000	$5s^25p^4\ ^1D_2$	$5p^36s\ ^3D_3$	1.25E+09	1.33E-01	0.042
38	327.760	327.7600	0.000	$5s^25p^4\ ^1D_2$	$5p^36s\ ^3D_1$	2.16E+09	1.02E-01	0.035
170	329.744	329.7480	-0.004	$5s^25p^4\ ^3P_0$	$5p^36s\ ^3S_1$	7.40E+09	3.54E-01	0.027
18	331.353	331.3490	0.004	$5s^25p^4\ ^1D_2$	$5p^36s\ ^3D_2$	1.40E+09	1.12E-01	0.051
25	341.580	341.5720	0.008	$5s^25p^4\ ^3P_1$	$5p^36s\ ^3S_1$	3.00E+09	1.53E-01	0.037
65	571.236	571.2370	-0.001	$5s^25p^4\ ^3P_2$	$5s5p^5\ ^3P_1$	9.58E+08	1.40E-01	0.073
25	572.450	572.4390	0.011	$5s^25p^4\ ^1D_2$	$5s5p^5\ ^1P_1$	1.43E+09	2.09E-01	0.057
30	606.582	606.5820	0.000	$5s^25p^4\ ^3P_1$	$5s5p^5\ ^3P_0$	1.19E+09	6.61E-02	0.069
75	611.894	611.8940	0.000	$5s^25p^4\ ^3P_2$	$5s5p^5\ ^3P_2$	8.40E+08	2.36E-01	0.076
20	621.703	621.7030	0.000	$5s^25p^4\ ^3P_0$	$5s5p^5\ ^3P_1$	3.35E+08	5.82E-02	0.036
30	665.114	665.1110	0.003	$5s^25p^4\ ^3P_1$	$5s5p^5\ ^3P_1$	2.46E+08	4.83E-02	0.070
15	704.617	704.6190	-0.002	$5s^25p^4\ ^1D_2$	$5s5p^5\ ^3P_1$	8.51E+07	1.91E-02	0.080
45	720.884	720.8800	0.004	$5s^25p^4\ ^3P_1$	$5s5p^5\ ^3P_2$	2.67E+08	1.03E-01	0.093
10	721.828	721.8350	-0.007	$5s^25p^4\ ^1S_0$	$5s5p^5\ ^1P_1$	9.03E+07	2.08E-02	0.150
25	767.520	767.5240	-0.004	$5s^25p^4\ ^1D_2$	$5s5p^5\ ^3P_2$	1.18E+08	5.27E-02	0.087

*: The intensities and the observed wavelengths are from Tauheed et al. [6]

4. Summaries

This work presents the extensive calculations for the level energies and transitions rates of six times ionized cerium (Ce VII). Using the GRASP2018 [9], we describe 5 even parity states, from $5s^25p^4$ configuration, and 14 odd parity states, from $5s5p^5$ and $5p^36s$ configurations by spectral study of Ce VII from MCDHF calculations. The obtained energies are in good agreement with available experimental data [6].

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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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