Journal of Atomic, Molecular, Condensate & Nano Physics
Vol. 7, No. 1, pp. 35–40, 2020
ISSN 2349-2716 (online); 2349-6088 (print)
Published by RGN Publications

http://www.rgnpublications.com

DOI: 10.26713/jamcnp.v7i1.1364

The Multi-configuration Dirac-Hartree-Fock Calculations for Cs VII

Research Article

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Abstract. Theoretical energy levels, wavelengths and transitions probabilities ofsix-times ionized cesium (CsVII) are calculated using multi-configuration-Dirac-Hartree-Fock (MCDHF) method. The present calculations have been performed for the $5s^25p$, $5s^26s$, $5s^25d$, $5s5p^2$configurations using the GRASP2018 package. The electron correlation effects, Breit interaction and quantum electrodynamics effects have been considered in the calculations.

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

PACS. 32.30.-r; 33.2.Ni; 34.80.Dp; 31.15.Ne

Received: February 22, 2020 **Accepted:** April 4, 2020

1. Introduction

In six times ionized cesium (Cs VII) the ground configuration is $5s^25p$ and the low-excited configurations are $5s5p^2$, $5s^25d$ and $5s^26s$. Forthis ion the experimental energy values and wavelengths are available in NIST database [8]. These data were prepared by Sansonetti in 2009 [10] based on the original observations from Gyasov and Joshi [5]. They did observe 184 lines and established 69 energy levels for this spectrum. For many applications particularly in Astrophysical observations and plasma diagnostics, transition parameters (transition probabilities, oscillator strengths and line-strengths) data are quite important. However, no such data are available for this spectrum except the one for the forbidden line between the $^2P_{1/2,3/2}$ levels of the ground $5s^25p$ configuration [9, 11].

In this work we have investigated theoretical energy levels, wavelengths and transition probabilities with a fully relativistic MCDHF approach applied for the $5s^25p$, $5s^26s$, $5s^25d$ and $5s5p^2$configurations. We also carried out a separate calculation to determine the transition parameters of the forbidden line $5s^25p\ ^2P_{1/2}–^2P_{3/2}$ between the ground levels. The two wavelengths associated with the forbidden lines (M1 and E2) superimposing each other are very weak transitions, though M1 is the dominant component while electric quadrupole transition E2 is much weaker, resulting long lifetime of theupper level$^2P_{3/2}$.

2. Relativistic MCDHF Calculations

The computer code GRASP2018 is based on multi-configuration Dirac-Hartree-Fock method (MCDHF). The full description of the theoretical methods has been discussed elsewhere [2, 3]. Consequently, we only bring in the necessary features of it. 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

$$\psi(\Gamma PJM) = \sum_r C_r \phi(\gamma_r PJM)$$

where C_r is the configuration mixing coefficients, P, J and M are the parity, total angular momentum and magnetic quantum numbers, respectively. The CSFs are the linear combination of Slater determinant constructed from the relativistic orbitals. The agreement between transition rates computed in length (Babushkin gauge) and velocity (Coulomb gauge) form reflects the accuracy of our results. The relative difference can be used as an indicator of uncertainty dT [1] defined as:

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

$$\psi(\Gamma PJM) = \sum_r C_r \phi(\gamma_r PJM).$$

The calculations have been done parity-wise consequently the odd and even states were determined in separate calculations in the extended optimization level (EOL) scheme. The calculations of odd states were based on the CFS expansion formed by $5s^25p$ configuration and of even state from $5s5p^2$, $5s^26s$ and $5s^25d$ configurations define the multi-reference (MR) set. Energy levels, oscillator strengths and transition probabilities for electric-dipole (E1) and magnetic-dipole(M1) have been calculated through large configuration state function expansions for $n = 8$ complex within the framework of multi-configuration Dirac-Fock method (MCDHF). During the calculation transverse photon interaction in the low frequency limit, vacuum polarization and self energy corrections was considered. The valance electron correlation effects are accounted for expansions obtained from CSFs through single-double multi-reference (SD-MR) expansions to increase active sets of orbitals [7].

3. Results and Discussion

In the MCDHF calculations, the CSFs are obtained with the MR set of $5s^25p$ configuration state in odd parity system and, $5s5p^2$, $5s^25d$, $5s^26s$ configurations state in even parity matrix. The active set is increase in step of orbital layers and the configuration expansions then obtained by single-double (SD) substitutions from the multi-reference (MR) set to active set of orbitals for principal quantum number up to $n = 8$ for orbital angular momenta up to $l = 2$ and, $n = 5$ for $l = 3$ and 4. The valance effects are taken into account for 8s, 8p, 8d, 5f, 5g while keeping the core ($1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}$) frozen. Breit Interaction (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 theoretically calculated energy levels along with their experimental values are given in Table 1. The wavelengths and A-values for the allowed (E1) $5s^25p$-{$5s5p^2$, $5s^2$(5d+6s)} transitions are provided in Table 2. To our knowledge, this is the first MCDHF calculations for Cs VII spectrum. The calculated transition rates for the forbidden line $5s^25p\ ^2P_{1/2}$-$^2P_{3/2}$, and corresponding lifetime of $5s^25p^2P_{3/2}$ level are given in Table 3. The present results of M1 and E2 are in good agreement with those reported by Wang [11] and by Safronova et al. [9].

Table 1. Energy levels of Cs VII

Configuration	Level	$E_{MCDHF}{}^a$ (cm^{-1})	$E_{exp}{}^b$(cm^{-1})
$4d^{10}.5s^2.5p$	$^2P^\circ_{1/2}$	0.00	0
$4d^{10}.5s^2.5p$	$^2P^\circ_{3/2}$	18768.98	19379.3
$4d^{10}.5s.5p^2.(^3P)$	$^4P_{1/2}$	100258.17	104226.2
$4d^{10}.5s.5p^2.(^3P)$	$^4P_{3/2}$	109641.95	114254.9
$4d^{10}.5s.5p^2.(^3P)$	$^4P_{5/2}$	118380.56	122261.3
$4d^{10}.5s.5p^2.(^1D)$	$^2D_{3/2}$	144889.90	141168.5
$4d^{10}.5s.5p^2.(^1D)$	$^2D_{5/2}$	149304.97	147182.2
$4d^{10}.5s.5p^2.(^3P)$	$^2P_{1/2}$	168074.50	158091.3
$4d^{10}.5s.5p^2.(^1S)$	$^2S_{1/2}$	190688.98	178190.9
$4d^{10}.5s.5p^2.(^3P)$	$^2P_{3/2}$	199179.19	179339.4
$4d^{10}.5s^2.5d$	$^2D_{3/2}$	226384.91	205994.2
$4d^{10}.5s^2.5d$	$^2D_{5/2}$	229389.19	208786.9
$4d^{10}.5s^2.6s$	$^2S_{1/2}$	279870.23	273351.5

^{a}: Energy levels calculated by fully relativistic approach (MCDHF)
^{b}: Energy levels experimentally reported in NIST ASD

Table 2. Calculated electric dipole (E1) transition probabilities of Cs VII lines

Configuration	Level	Configuration	Level	λ (Å)	S_L[a]	A_L[a] (s^{-1})	S_V[a]	A_v[a] (s^{-1})	dT[b]
$4d^{10}.5s^2.5p$	$^2P_{1/2}$	$4d^{10}5s^26s$	$^2S_{1/2}$	357.31	3.09E-01	6.87E+09	2.90E-01	6.45E+09	0.06198
$4d^{10}.5s^2.5p$	$^2P_{3/2}$	$4d^{10}5s^26s$	$^2S_{1/2}$	382.99	8.82E-01	1.59E+10	8.13E-01	1.47E+10	0.07816
$4d^{10}.5s^2.5p$	$^2P_{1/2}$	$4d^{10}.5s^2.5d$	$^2D_{3/2}$	441.73	4.47E+00	2.63E+10	3.96E+00	2.33E+10	0.11439
$4d^{10}.5s^2.5p$	$^2P_{3/2}$	$4d^{10}.5s^2.5d$	$^2D_{5/2}$	474.79	9.25E+00	2.92E+10	8.07E+00	2.55E+10	0.12693
$4d^{10}.5s^2.5p$	$^2P_{3/2}$	$4d^{10}.5s^2.5d$	$^2D_{3/2}$	481.66	1.57E+00	7.10E+09	1.35E+00	6.14E+09	0.13507
$4d^{10}.5s^2.5p$	$^2P_{1/2}$	$4d^{10}.5s.5p^2$	$^2P_{3/2}$	502.06	1.50E+00	6.00E+09	1.24E+00	4.96E+09	0.17198
$4d^{10}.5s^2.5p$	$^2P_{1/2}$	$4d^{10}.5s.5p^2$	$^2S_{1/2}$	524.41	1.26E+00	8.86E+09	1.02E+00	7.14E+09	0.19411
$4d^{10}.5s^2.5p$	$^2P_{3/2}$	$4d^{10}.5s.5p^2$	$^2P_{3/2}$	554.29	6.57E+00	1.95E+10	5.38E+00	1.60E+10	0.18015
$4d^{10}.5s^2.5p$	$^2P_{3/2}$	$4d^{10}.5s.5p^2$	$^2S_{1/2}$	581.67	2.29E+00	1.18E+10	1.93E+00	9.92E+09	0.1594
$4d^{10}.5s^2.5p$	$^2P_{1/2}$	$4d^{10}.5s.5p^2$	$^2P_{1/2}$	594.97	2.09E+00	1.00E+10	1.78E+00	8.54E+09	0.14913
$4d^{10}.5s^2.5p$	$^2P_{1/2}$	$4d^{10}.5s.5p^2(^1D_2)$	$^2D_{3/2}$	690.18	1.35E+00	2.07E+09	1.23E+00	1.90E+09	0.0826
$4d^{10}.5s^2.5p$	$^2P_{3/2}$	$4d^{10}.5s.5p^2$	$^2P_{1/2}$	669.77	1.30E-01	4.38E+08	1.37E-01	4.63E+08	0.05381
$4d^{10}.5s^2.5p$	$^2P_{3/2}$	$4d^{10}.5s.5p^2(^1D_2)$	$^2D_{5/2}$	766.07	1.44E+00	1.08E+09	1.37E+00	1.03E+09	0.05283
$4d^{10}.5s^2.5p$	$^2P_{3/2}$	$4d^{10}.5s.5p^2(^1D_2)$	$^2D_{3/2}$	792.89	1.86E+03	1.89E+06	6.08E-03	6.18E+06	0.69344
$4d^{10}.5s^2.5p$	$^2P_{1/2}$	$4d^{10}.5s.5p^2(^3P_2)$	$^4P_{3/2}$	912.06	2.89E-03	1.93E+06	3.27E-03	2.18E+06	0.11637
$4d^{10}.5s^2.5p$	$^2P_{1/2}$	$4d^{10}.5s.5p^2(^3P_2)$	$^4P_{1/2}$	997.42	6.21E-02	6.34E+07	5.27E-02	5.38E+07	0.15041
$4d^{10}.5s^2.5p$	$^2P_{3/2}$	$4d^{10}.5s.5p^2(^3P2)$	$^4P_{5/2}$	1003.9	1.73E-01	5.77E+07	1.64E-01	5.46E+07	0.05303
$4d^{10}.5s^2.5p$	$^2P_{3/2}$	$4d^{10}.5s.5p^2(^3P_2)$	$^4P_{3/2}$	1100.44	1.91E-02	7.27E+06	1.46E-02	5.56E+06	0.23497
$4d^{10}.5s^2.5p$	$^2P_{3/2}$	$4d^{10}.5s.5p^2(^3P_2)$	$^4P_{1/2}$	1227.16	2.61E-02	1.43E+07	2.66E-02	1.46E+07	0.2034

[a] Line strength and transition rates in length (S_L, A_L) and velocity (S_V, A_V) forms.

[b] Fractional uncertainty indicator for the transition rate.

Table 3. Transition rate (A-value in s^{-1}) for the forbidden line$5s^25p\ ^2P_{1/2}$-$^2P_{3/2}$

λ_{calc}, (Å)	λ_{exp} (Å)	Type	A-value (s^{-1})			$^2P_{3/2}$ Lifetime (ms)	
			Original[a]	Scaled[a]	Others	This work	Others
5242.314	5160.15	M1	62.10	65.12	65.15 [11], 65.10 [9]	15.215	15.182 [11], 15.20 [9]
5242.313	5160.15	E2	0.5593	0.6054	0.7180 [11], 0.6371 [9]		

[a] The original values are the present work from the MCDHF method, scaled to the experimental wavelength for the comparison purpose

4. Conclusions

In this work we have calculated the energy levels and transitions of the array $5s^2$5p-{5s$5p^2$, $5s^2$(5d+6s)} for Cs VII by a fully relativistic multi-configuration-Dirac-Hartree-Fock (MCDHF) method. Transition parameters for a total of 21 transitions; 19 for E1 type, one each for M1 and E2of Cs VII are given in Tables 2 and 3.

Acknowledgements

AW and AHare thankful to the University Grants Commission of India for financial assistance and department of physics Aligarh Muslim University for providing facilities for this work. Discussions held with Dr. Haris K. are greatly appreciated.

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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