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Stellar And Interstellar Transition Lines Of C IV, N V And O VI

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ABSTRACT

In this paper, we study the parameters of allowed and forbidden transition lines for lithium-like ions (C IV, N V, and O VI), which are vital for understanding the dynamics, internal temperatures, densities, and chemical abundances of stellar atmospheres and the interstellar medium (ISM). Using the Relativistic Coupled-Cluster (RCC) method incorporating single, double, and partial triple excitations (CCSD(T)) alongside the Dirac-Coulomb-Breit (DCB) Hamiltonian, the we calculate core correlation energies, ionization potentials, oscillator strengths, and hyperfine structures. The accuracy of the generated atomic wavefunctions is confirmed by the close agreement between the length and velocity gauges of the reduced electric dipole (E1) matrix elements.

INTRODUCTION

Parameters of transition lines of C VI, N V and O VI are important to understand the dynamics and nature of stellar atmosphere and interstellar medium (ISM) (Ferrero et al. 2012; de Avillez et al. 2012; Prochaska et al 2011; Fox 2011; Barstow et al. 2010). There have been long literature on the applications of resonance lines (1548 Å, 1550 *Å* for C IV; 1238 *Å,* 124200C Å for N V; 1032 *Å,* 1038 *Å* for O VI) (NIST; Peach et al 1988), though forbidden lines provides very crucial parameters of these astronomical bodies (Chen et al. 2010; Burgess et al. 1998). Knowledge of forbidden (E2 and M1) transition probabilities and hyperfine-structure splitting is important for the estimations of density and internal temperature measurements in low density hot plasmas. Accurate estimations of these transition rates are extremely important to characterize the astronomical emission region (Qu et al. 1999). We have studied of electric dipole and quadrupole transition rates of these ions using relativistic coupled cluster (RCC) method based on Dirac-Coulomb-Breit (DCB) Hamiltonian (Dutta and Majumder 2012, Mondal et al. 2013). These are the augmented calculation of Sur and Chaudhuri (Sur and Chaudhuri 2007) who had calculated branching ratio of transitions from 4*s*-state only using CC method based on Dirac-Coulomb Hamiltonian.

Though significance of Breit interaction is small for the transition rates, but they will be significant for hyperfine effects on the low-lying states of these ions. Since the launching of high-resolution space telescopes, the accurate study hyperfine structures become extremely important. Closed observed lines (Jonsson 2007) are needed to include the effect in the theoretical modelling of the line profiles (Kurucz 1993; Huehnermann 1993). Mostly non-relativistic many-body approaches had been used with relativistic correction for ground state hyperfine splitting of few of these ions (Shabaev et al. 1997; Gaun et al.1998).

The RCC method with single, double and partial triple excitation (CCSD(T)) have been employed here which takes into account higher order correlations exhaustively. In the present paper, we have calculated the ionization potentials and oscillator strength of electric dipole (E1) transitions and compare them with NIST results (NIST, Ralchenko et al. 2012). The transition probabilities of forbidden transitions (electric quadrupole only as magnetic dipole transition are very weak) between these states for C IV, O V, and N VI. To estimate the accuracy of our calculations of hyperfine splitting of these states, we have compared the length and velocity gauge E1 matrix elements for few relevant transitions as radial parts of both the matrices have same format. Panigrahy et al. (Panigrahy et al. 1989) have used the relativistic many-body perturbation theory to study different correlation mechanisms on the magnetic dipole hyperfine constant (A) of Li-like systems.

THEORY

A. Rleativistic Coupled-cluster theory

According to the RCC theory, the correlated single valence atomic state wave-function ($|\psi_v\rangle$) having valance orbital 'v' can be expanded in terms of Dirac-Fock (DF) orbital ($|\varphi_v\rangle$) as given below:

$|\psi_v> = e^T \{1+S_v\}|\varphi_v>$ (1)

Here, T is the closed shell cluster operator which considers excitations from the core orbitals only and S_v is the open shell cluster operator corresponding to the valance electron v (Gopakumar et al. 2001). The cluster amplitudes have been calculated from the RCC equation based on DCB Hamiltonian.

B. Hyperfine Splitting

Hyperfine interaction is the non-central interaction between the electrons and the electromagnetic multi-pole moments of the nucleus. The Hamiltonian of interaction is often written as,

$$Hhfs = \sum_k T^k.M^k \quad (7)$$

Where $T^{(k)}$ and $M^{(k)}$ are spherical tensor operators of rank k in the electronic and nuclear spaces respectively. Here, $k = 1,2,3$ represents the terms which arise from different nuclear moments like magnetic dipole, electric quadrupole, magnetic octupole respectively. The magnetic dipole contribution dominates over others. So, we can restrict the above summation for only $k = 1$ and this leads to

$H_{hfs} = T(1).M(1)$ (8)

The above expression gives the hyperfine energy splitting

$$\Delta E = A_J \langle I \cdot J \rangle = \frac{1}{2} A_J \left[F(F+1) - J(J+1) - I(I+1)\right] \quad (9)$$

where hyperfine interaction constant is derived as

$$A_j = \frac{g_I \mu_N < \gamma J \,||T^{(1)}|| \,\gamma J >}{\sqrt{J(J+1)(2J+1)}} \quad (10)$$

RESULTS AND DISCUSSIONS

The generations of accurate atomic wavefunctions in the RCC level of calculations largely depends on the precise estimation of the DF orbital wavefunctions. The latter type of orbital wavefunction is generated in the environment with two core electrons at 1s orbital. The radial part of these wavefunctions is expressed in terms of universal Gaussian type basis having two optimized parameters α_0 and β for exponents. 30, 25, 20, and 20 are the number of bases for s, p, d, and f symmetries, respectively. In order to choose these parameters, the energies and wavefunctions of the orbital bases are optimized with respect to the same as obtained from the GRASP2 code (Parpia et al. 2006). For C IV, O V and N VI, these exponential parameters are chosen as 0.005825, 2.73), (0.003265, 2.73) and (0.00525, 2.73), respectively. At the RCC level of calculations, the number of orbial bases for s, p, d and f symmetries are restricted up to 12, 11, 10 and 10 for C IV and O V and 13, 12, 10 and 10 for N VI, respectively depending on the consistency of the numerical convergence of core correlation energies with increasing number of bases.

The calculated ionization potentials of the ground state $2s^2S_{1/2}$ for C IV, N V and O VI are estimated to be 520144.554, 789493.57 and 1113968.18 cm^{-1}, respectively, which are in well agreement with the NIST results (520178.4, 789537.2 and 1114004 cm^{-1}, respectively). The RCC excitation energies of the different atomic states deviate about 0.05%, 0.06% and 0.06% from the NIST values (Ralchenko et al. 2011) for the ions C IV, N V and O VI, respectively. Further verification of the accuracy of the wavefunction of the atomic states are done by checking agreements between E1 reduced transition matrix elements in the form of length and velocity gauges.

The oscillator strengths of E1 transitions are calculated and compared to the NIST. The average deviation of our calculations is 1.7% and agree well with recently calculated results using SUPERSTRUCTURE code whose values of 3% off from the NIST results.

Table 1:: Hyperfine constant A_J in MHz and hyperfine energy splitting in MHz

state		*CIV*			N_v			*OVI*	
J	A_J	*F*	ΔE	A_J	*F*	ΔE	A_J	*F*	ΔE
2 $2S_{\frac{1}{2}}$	5615.587	1	1403.897	-3961.936	1	-990.484	-8458.092	3	-10572.615
		0	-4211.690		0	2971.452		2	14801.661
2 $2P^o_{\frac{1}{2}}$	1394.302	1	348.576	-1038.599	1	-259.650	-2303.319	3	-2879.149
		0	-1045.727		0	778.950		2	4030.808
2 $2P^o_{\frac{3}{2}}$	118.072	2	88.554	-107.676	2	-80.757	-270.437	4	-1014.138
		1	-147.590		1	134.595		1	1419.794
3 $2S_{\frac{1}{2}}$	1516.988	1	379.247	-1084.665	1	-271.166	-2354.602	3	-2943.252
		0	-1137.741		0	813.499		2	4120.553
3 $2P^o_{\frac{1}{2}}$	398.161	1	99.540	-296.578	1	-74.145	-659.012	3	-823.765
		0	-298.621		0	222.434		2	1153.271
state		***CIV***			$\boldsymbol{N_v}$			***OVI***	
J	A_J	*F*	ΔE	A_J	*F*	ΔE	A_J	*F*	ΔE
3 $2P^o_{\frac{3}{2}}$	39.365	2	29.523	-35.135	2	-26.351	-86.587	4	-324.703
		1	-49.206		1	43.919		1	454.584
3 $2D_{\frac{3}{2}}$	35.139	2	26.354	-27.616	2	-20.712	-63.634	4	-238.627
		1	-43.924		1	34.520		1	334.078
3 $2D_{\frac{5}{2}}$	13.941	3	17.426	-11.007	3	-13.758	-25.488	5	-159.300
		2	-24.396		2	19.262		0	223.020
4 $2S_{\frac{1}{2}}$	613.191	1	153.298	-442.663	1	-110.666	-1011.616	3	-1264.520

		0	-459.893		0	331.997		2	1770.328
$4\,2P^{o}_{\frac{1}{2}}$	159.528	1	39.882	-118.845	1	-29.711	-269.031	3	-336.290
		0	-119.646		0	89.134		2	470.805
$4\,2P^{o}_{\frac{3}{2}}$	16.655	2	12.492	-14.601	2	-10.951	-36.463	4	-136.738
		1	-20.820		1	18.251		1	191.433
$4\,2D^{o}_{\frac{3}{2}}$	15.006	2	11.254	-11.823	2	-8.867	-26.827	4	-100.601
		1	-18.757		1	14.778		1	140.841
$4\,2D^{}_{\frac{5}{2}}$	5.8172	3	7.271	-4.615	3	-5.769	-10.548	5	-65.926
		2	-10.180		2	8.077		0	92.296
$4\,2F^{o}_{\frac{5}{2}}$	4.409	3	5.511	-3.471	3	-4.338	-8.028	5	-50.175
		2	-7.716		2	6.073		0	70.244
$4\,2F^{o}_{\frac{7}{2}}$	2.445	4	4.278	-1.924	4	-3.367	-4.449	6	-38.932
		3	-5.500		3	4.328		1	50.056

4. CONCLUSION

We have studied the allowed and forbidden transitions lines of C IV, N V and O VI belong to the Li-isoelectronic sequence using coupled-cluster method with relativistic corrections. To check the accuracy of the calculations, length and velocity gauges of the reduced matrix elements of the electric dipole operator has been calculated and a good agreement is found between them. Our calculated oscillator strengths agree well with the other theocratical and experimental results found in the literature. These E1 transitions, fall in the infrared, visible and ultraviolet regions, are important in density estimations in different astronomical systems. The major aspect of this work is the calculations of the forbidden transition probabilities of astrophysical importance which is the first time in the literature with best of our knowledge. Strong transition lines between the $3d^2D$ multiplate and ground states has been reported. These lines can be used in future as a tool of exploration of internal temperature and abundances of the species in astrophysical plasmas.

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REFERENCES

1. Ferrero R F , Dura C M, Halbwachs J -L and Cubeiro A M C 2012¨ *The Astronomical Journal* 143 28

2. de Avillez M A and Breitschwerdt D 2012 *Astronomy and Astrophysics* 2012 539 L1,
3. Prochaska J. Xavier, Weiner B, Chen H -W, Mulchaey J, and Cooksey K 2011 *The Astrophysical Journal* 740 91
4. Fox A J 2011 *The Astrophysical Journal* 730 58.
5. Barstow M A, Boyce D D, Welsh B Y, Lallement R, Barstow J K, Forbes A E, Preval S 2010 *The Astrophysical Journal* 723 1762.
6. Henley D B, Kwak K, Shelton R L 2012 *The Astrophysical Journal* 753 58.
7. Peach G, Saraph H E, and Seaton M J 1988 *J. Phys. B* 21 3669.
8. Chen C -Y, Wang K , Huang M , Wang Y -S and Zou Y -M 2010 *Journal of Quantitative Spectroscopy and Radiative Transfer* 111 6.
9. Burgess A, Chidichimo -M C, Tully -J A 1998 *Astron. Astrophys. Suppl. Ser.* 131.
10. Sur C, Chaudhuri R K 2007 *J. Phys. B: At. Mol. Opt. Phys.* 40 4307. Jonsson P, 2007¨ *J. Phys.: Conf. Ser.* 72 012011.
11. Kurucz R L 1993 *Physica Scripta T* 47.
12. Huehnermann H 1993 *Physica Scripta T* 47.
13. Shabaev V M, Shabaeva M B, Tupitsyn I I 1997 *Astronomical and Astrophysical Transactions* 12.
14. Gaun X -X, Wang Z -W 1998 *Eur. Phys. J. D* 2 21.
15. Gopakumar G, Merlitz H, Majumder S, Chaudhuri R K, and Das B P 2001 *Phys. Rev. A* 64 032502
16. Sahoo B K, Majumder s, Merlitz H, Chaudhuri R K, Das B P, and Mukherjee D 2006 *J. Phys. B* 39 355.
17. Qu L, Wang Z, Li B 1999 *Eur. Phys. J. D.* 5 173-177.
18. Ralchanko Y, Kramida A E, Reader J, and NIST ASD TEAM(2011) *NIST Atomic Spectra Database* version 4.1.0; available at [http://physics.nist.gov/asd][2012, June 20]
19. Panigrahy S N, Dougherty R W, Das T P, and Andriessen J 1989 *Phys. Rev. A* 40 1765.
20. Parpia F A, Fischer C F, Grant I P 2006 *Comput. Phys.Commun.* 175 745
21. Dutta N N, Majumder S 2012 *Phys. Rev. A* 85 032512.
22. Dutta N N, Majumder S 2011 *The Astrophysical Journal* 737 25.
23. Mondal P K, Dutta N N, Dixit G, Majumder S 2013 PHYSICAL REVIEW A 87, 062502