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# Atomic structure of the carbon like ion Ca XV

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**Abstract.** Energy levels, oscillator strengths and transition probabilities for the multicharged carbon like Ca XV ion have been calculated using the pseudo-relativistic Hartree-Fock (HFR) approach using the new Cowan atomic structure code 2018. Results have been compared with NIST datdabase and other calculated data. There are great lack on atomic structure data of Ca XV and obtained new data will be important for plasma diagnostic and astrophysical modeling.

**Key words:** spectral lines – energy levels – oscillator strengths –transition probabilities

## 1. Introduction

Carbon-like ions are highly abundant elements and their lines are prominent in both stellar and interstellar spectra and they are interesting for possible astrophysical plasma diagnostic applications (Al-Modlej *et al.*, 2018). One example of them is calcium (Ca) which has a nuclear charge Z=20 and it has cosmic abundances in astrophysical spectra (Träbert *et al.*, 2018). Carbon-like ions are also important for investigation in plasma physics, fusion research and plasma technologies.

In general, we can obtain ionized calcium by Tokamaks which are proven light sources suitable for measuring spectra of astrophysical relevance (Träbert *et al.*, 2018), as well as by the solar flare plasma where Extreme Ultra-Violet (EUV) solar emission lines of highly ionized calcium have been recorded (Nahar, 2017).

Indeed, what is interesting now is the study of Ca XV, a highly charged carbon-like ion that typically exists in high temperature plasmas and plays an important role for diagnostics and modeling.

Researchers have done some important experimental studies on spectral lines of Ca XV where the diagnostic potential of these lines was noted. It is worth mentioning that the data on atomic properties are not only relevant to spectroscopy, but these values are of interest in a variety of other fields in physics and technology (Colón and Alonso-Medina, 2010). As an example, the diagnostic emission lines have been frequently observed in solar EUV spectra of carbon-like Ca XV by Dere (1978). Moreover, Ca XV was detected in the Extreme-Ultraviolet Explorer satellite spectrum of the star $\xi$ Bootis A (Laming and Drake, 1999). Also, EUV emission lines of Ca XV in solar and laboratory spectra were studied by Keenan *et al.* (2003).

Recently, the most important experimental study in this field was by Trbert et al. (2018), where they investigated the emission line intensity pattern of highly charged Ca and Ar in the EUV in a laboratory plasma, by using a Tokamak plasma discharge in hydrogen carrying some Ar and intermittently seeded with Ca. The task is done injecting these elements by laser pulse into a plasma dominated by hydrogen. Fortunately, the results of the study of spectrum for Ca produced a fair number of spectral lines. The data of this experimental study have been compared with databases especially CHIANTI (Dere *et al.*, 2019). Most importantly, they found that Ca XV is particularly rich in lines in the EUV spectral range and the strongest line was $2s^2\ 2p^2\ {}^1D_2$ - $2s\ 2p^3\ {}^1D^o_2$ at $\lambda = 161.1$ Å.

In the present work, we calculated energy levels for the configuration expansion: $2s^2\ 2p^2$, $2s^2\ 2p\ 3p$, $2s^2\ 2p\ 4p$, $2s\ 2p^3$, $2s^2\ 2p\ 3s$, $2s^2\ 2p\ 4s$, $2s^2\ 2p\ 5s$ and $2s^2\ 2p\ 3d$. Also, we computed oscillator strengths and transition probabilities corresponding to some spectral lines of the carbon like Ca XV ion using a relativistic configuration interaction method based on numerical wave functions calculated with a single configurations Hartree-Fock Relativistic (HFR) approach including core-polarization potential and the corresponding corrections in the matrix elements because for any system considered, complex like Ca XV ion, both relativistic and correlation effects could be relevant. So, all our calculations were in the framework of the HFR by means of a recent version of the Cowan computer code adapted by Kramida (2018).

We describe in Section 2 the theoretical calculations and then in Section 3 the results of the atomic structure of Ca XV ion. The conclusions are presented in Section 4.

## 2. Hartree-Fock Relativistic method

For the hydrogen atom, the Schrödinger equation is solved exactly, but for a system consisting of a multi-electron atom or molecule, we must use approx-

imate methods such as the HFR method, where the Schrödinger equation for $N$-electrons atom wavefunction can be written as:

$$\left[\sum_{i=1}^{N}\left(-\tfrac{1}{2}\nabla_{r_i}^2-\tfrac{Z}{r_i}\right)+\sum_{i<j}^{N}\tfrac{1}{r_{ij}}\right]\Psi(q_1,q_2,\ldots,q_N)=E\Psi(q_1,q_2,\ldots,q_N) \tag{1}$$

where $q_i$ denotes the set of the discrete spin variable of electron $i$ and continuous spatial coordinates $r_i$.

In this method, the many wave functions are written as a linear superposition of products of single-particle spin orbitals wave functions but these wave functions, anti-symmetric for $N$-electrons, must satisfy the Pauli principle. So, this product is written as a determinant known as the Slater Determinant (Bransden & Joachain, 2003):

$$\Psi(q_1,q_2,\ldots,q_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix} u_\alpha(q_1) & u_\beta(q_1) & \cdots & u_\nu(q_1)\\ u_\alpha(q_2) & u_\beta(q_2) & \cdots & u_\nu(q_2)\\ \vdots & \cdots & \cdots & \vdots\\ u_\alpha(q_N) & u_\beta(q_N) & \cdots & u_\nu(q_N)\end{vmatrix} \tag{2}$$

The functions $u_\lambda(q_i)$ satisfy the HartreeFock Relativistic equation (Al-Towyan *et al.*, 2016; Colón and Alonso-Medina, 2010):

$$\begin{aligned}\left[-\tfrac{1}{2}\nabla_{r_i}^2-\tfrac{Z}{r_i}\right]u_\lambda(q_i)+\left[\sum_\mu\int u_\mu^*(q_i)\tfrac{1}{r_{ij}}u_\mu(q_j)dq_j\right]u_\lambda(q_i)\\ -\left[\sum_\mu\int u_\mu^*(q_j)\tfrac{1}{r_{ij}}u_\lambda(q_j)dq_j\right]u_\lambda(q_i)=E_\lambda u_\lambda(q_i)\end{aligned} \tag{3}$$

where $\lambda,\mu=\alpha,\beta,\ldots,\nu$ and the summation over $\mu$ extends over the $N$ occupied spin-orbitals.

We note from Eq. (2) that the determinant vanishes if two electrons are the same. That means the Hartree wavefunction is anti-symmetric with respect to the interchange of any set of space-spin coordinates of any two particles, but its Hamiltonian must be invariant under this condition. From here it was necessary to introduce the relativistic corrections with a Breit-Pauli Hamiltonian including mass-variation term, one-body Darwin term and Blume-Watson spin-orbit term which contain the part of the Breit interaction that can be reduced to a one-body operator, also treated by the perturbation theory Alonizan *et al.* (2016).

In previous works (Alonizan *et al.* (2016), for example), we obtained better results with HFR method comparing to similar methods as TFDA potential method; which gives advantage of this method.

The Cowan (CW) code, a suite of four atomic structure programs (RCN, RCN2, RCG and RCE) version 2018 (Kramida, 2018), uses this HFR method. The three first codes are for *ab initio* atomic structure calculations and the

fourth one (RCE) is used to have least-squares fit calculations using an iterative procedure (Cowan, 1981).

## 3. Atomic structure of the ion Ca XV

We performed calculations of energy levels for the carbon-like ion Ca XV by the suite of atomic structure codes of Cowan adapted by Kramida (2018). The configuration expansion of the basis set used in this work consists of 3 even parity configurations: $2s^2\ 2p^2$ and $2s^2\ 2p\ np$ ($n$=3,4) and 5 odd parity configurations: $2s\ 2p^3$, $2s^2\ 2p\ ns$ ($n$=3,4,5) and $2s^2\ 2p\ 3d$.

The calculated values of energy levels and oscillator strengths obtained with this code have been compared with other theoretical methods (Ekman *et al.*, 2014), and with data from NIST database (Kramida *et al.*, 2018).

### 3.1. Energy levels of the ion Ca XV

In Tables 1 to 5, we list energy levels of the configurations $2s^2\ 2p^2$, $2s\ 2p^3$, $2s^2\ 2p\ ns$ ($n = 3, 4, 5$), $2s^2\ 2p\ np$ ($n = 3, 4$), $2s^2\ 2p\ 3d$ for Ca XV ion. The obtained values are compared with those of NIST atomic database (Kramida *et al.*, 2018) and with Ekman *et al.* (2014) values which are calculated using the Multi-Configuration Hartree-Fock (MCHF) method.

**Table 1.** "Energy levels for the configuration $2s^2\ 2p^2$ of Ca XV." E(NIST) are from NIST database, E(CW) are the energy levels calculated by using the Cowan (CW) code, and E(EK) calculated using (MCDHF) by Ekman *et al.* All energies are in $cm^{-1}$.

| Conf. | Term | J | E(NIST) | E(CW) | E(EK) |
|---|---|---|---|---|---|
| $2s^2\ 2p^2$ | $^3P$ | 0 | 0 | 0 | 0 |
| $2s^2\ 2p^2$ | $^3P$ | 1 | 17559 | 16353 | 17553 |
| $2s^2\ 2p^2$ | $^3P$ | 2 | 35923 | 35171 | 35920 |
| $2s^2\ 2p^2$ | $^1D$ | 2 | 108600 | 104491 | 108736 |
| $2s^2\ 2p^2$ | $^1S$ | 0 | 197670 | 214620 | 197839 |

For the configuration $2s^2\ 2p^2$, CW code gives close to results to NIST. The results differ by about 4% from the NIST values, while, Ekman *et al.* values are very close to the NIST database values by 0.1%.

For the configuration $2s\ 2p^3$, the CW code gives values 5.6% higher than NIST database. Ekman *et al.* values are roughly the same differing by only 0.02% from the NIST ones.

**Table 2.** Same as Table 1, but for configuration 2s $2p^3$ of Ca XV.

| Conf. | Term | J | E(NIST) | E(CW) | E(EK) |
|---|---|---|---|---|---|
| 2s $2p^3$ | $^5S^o$ | 2 | 275900 | 311928 | 275788 |
| 2s $2p^3$ | $^3D^o$ | 3 | 500230 | 533862 | 500273 |
| 2s $2p^3$ | $^3D^o$ | 2 | 496680 | 529034 | 496724 |
| 2s $2p^3$ | $^3D^o$ | 1 | 497570 | 529652 | 497632 |
| 2s $2p^3$ | $^3P^o$ | 1 | 582780 | 607890 | 582942 |
| 2s $2p^3$ | $^3P^o$ | 2 | 585670 | 611053 | 585800 |
| 2s $2p^3$ | $^3P^o$ | 0 | 581730 | 606177 | 581886 |
| 2s $2p^3$ | $^1D^o$ | 2 | 729650 | 759011 | 730043 |
| 2s $2p^3$ | $^3S^o$ | 1 | 728880 | 757132 | 729176 |
| 2s $2p^3$ | $^1P^o$ | 1 | 814380 | 835599 | 814815 |

**Table 3.** Same as Table 1, but for configurations $2s^2$ 2p $n$s ($n = 3, 4, 5$) of Ca XV.

| Conf. | Term | J | E(NIST) | E(CW) | E(EK) |
|---|---|---|---|---|---|
| $2s^2$ 2p3s | $^3P^o$ | 0 | - | 4392032 | 4079795 |
| $2s^2$ 2p3s | $^3P^o$ | 1 | - | 4396297 | 4084845 |
| $2s^2$ 2p3s | $^3P^o$ | 2 | - | 4428144 | 4115926 |
| $2s^2$ 2p3s | $^1P^o$ | 1 | - | 4441352 | 4134012 |
| $2s^2$ 2p4s | $^3P^o$ | 0 | - | 4395728 | 5520070 |
| $2s^2$ 2p4s | $^3P^o$ | 1 | - | 4396731 | 5522133 |
| $2s^2$ 2p4s | $^3P^o$ | 2 | - | 4431652 | 5556429 |
| $2s^2$ 2p4s | $^1P^o$ | 1 | - | 4433840 | 5561725 |
| $2s^2$ 2p5s | $^3P^o$ | 0 | - | 4657441 | - |
| $2s^2$ 2p5s | $^3P^o$ | 1 | - | 4657861 | - |
| $2s^2$ 2p5s | $^3P^o$ | 2 | - | 4693386 | - |
| $2s^2$ 2p5s | $^1P^o$ | 1 | - | 4694256 | - |

For the configurations $2s^2$ 2p $n$s ($n = 3, 4, 5$) and $2s^2$ 2p $n$p ($n = 3, 4$) the NIST values do not exist for comparison. It should be noted that, we have obtained new energy values that do not exist in Ekman *et al.* for the configuration $2s^2$ 2p 5s and for the term $2s^2$ 2p 4p $^1$S.

**Table 4.** Same as Table 1, but for configurations $2s^2\ 2p\ np$ ($n = 3, 4$) of Ca XV.

| Conf. | Term | J | E(NIST) | E(CW) | E(EK) |
|---|---|---|---|---|---|
| $2s^2\ 2p3p$ | $^3S$ | 1 | - | 4476007 | 4257457 |
| $2s^2\ 2p3p$ | $^1P$ | 1 | - | 4446957 | 4228086 |
| $2s^2\ 2p3p$ | $^3D$ | 1 | - | 4424400 | 4205709 |
| $2s^2\ 2p3p$ | $^3D$ | 2 | - | 4445944 | 4229376 |
| $2s^2\ 2p3p$ | $^3D$ | 3 | - | 4472023 | 4255295 |
| $2s^2\ 2p3p$ | $^3P$ | 0 | - | 4475994 | 4250224 |
| $2s^2\ 2p3p$ | $^3P$ | 1 | - | 4494910 | 4270847 |
| $2s^2\ 2p3p$ | $^3P$ | 2 | - | 4501838 | 4276163 |
| $2s^2\ 2p3p$ | $^1D$ | 2 | - | 4528268 | 4314496 |
| $2s^2\ 2p3p$ | $^1S$ | 0 | - | 4567681 | 4361378 |
| $2s^2\ 2p4p$ | $^3S$ | 1 | - | 4491238 | 5618735 |
| $2s^2\ 2p4p$ | $^1P$ | 1 | - | 4487896 | 5612050 |
| $2s^2\ 2p4p$ | $^3D$ | 1 | - | 4450829 | 5572096 |
| $2s^2\ 2p4p$ | $^3D$ | 2 | - | 4456178 | 5583680 |
| $2s^2\ 2p4p$ | $^3D$ | 3 | - | 4488453 | 5613455 |
| $2s^2\ 2p4p$ | $^3P$ | 0 | - | 4459660 | 5590557 |
| $2s^2\ 2p4p$ | $^3P$ | 1 | - | 4455693 | 5582839 |
| $2s^2\ 2p4p$ | $^3P$ | 2 | - | 4491171 | 5619232 |
| $2s^2\ 2p4p$ | $^1D$ | 2 | - | 4496043 | 5631037 |
| $2s^2\ 2p4p$ | $^1S$ | 0 | - | 4501924 | - |

**Table 5.** Same as Table 1, but for configuration $2s^2\ 2p\ 3d$ of Ca XV.

| Conf. | Term | J | E(NIST) | E(CW) | E(EK) |
|---|---|---|---|---|---|
| $2s^2\ 2p3d$ | $^3F^o$ | 2 | 4363300 | 3951477 | 4363635 |
| $2s^2\ 2p3d$ | $^3F^o$ | 3 | 4379400 | 3963833 | 4378814 |
| $2s^2\ 2p3d$ | $^3F^o$ | 4 | - | 3988654 | 4401309 |
| $2s^2\ 2p3d$ | $^1D^o$ | 2 | - | 3966033 | 4385007 |
| $2s^2\ 2p3d$ | $^3D^o$ | 1 | 4399500 | 3975409 | 4402470 |
| $2s^2\ 2p3d$ | $^3D^o$ | 2 | 4411500 | 3991878 | 4413002 |
| $2s^2\ 2p3d$ | $^3D^o$ | 3 | 4426400 | 4000316 | 4425526 |
| $2s^2\ 2p3d$ | $^3P^o$ | 2 | 4435400 | 4006954 | 4433389 |
| $2s^2\ 2p3d$ | $^3P^o$ | 1 | 4434500 | 4008947 | 4435381 |
| $2s^2\ 2p3d$ | $^3P^o$ | 0 | - | 4010358 | 4436968 |
| $2s^2\ 2p3d$ | $^1F^o$ | 3 | 4475000 | 4032514 | 4474373 |
| $2s^2\ 2p3d$ | $^1P^o$ | 1 | 4473400 | 4032524 | 4475119 |

Moreover, with respect to the configuration $2s^2$ 2p 3d, some values of $^3F^o_4$, $^1D^o$ and $^3P^o_0$ terms in NIST database do not exist and for the existing data, the CW code gives results 9.6% higher than the NIST values but Ekman *et al.* values stays very close at the same rate from NIST. Indeed, we recommend the use of our CW results, because of the fact that we got new values with the CW code that are not present in the NIST database.

### 3.2. Oscillator strengths of the ion Ca XV

Instead of the absorption oscillator strengths $f_{ij}$ or the emission oscillator strengths $f_{ji}$, we use the weighted oscillator strengths $gf$:

$$gf = g_i f_{ij} = g_f f_{ji} \tag{4}$$

The weighted oscillator strengths and transition probabilities for selected allowed transitions $2s^2$ $2p^2$ $^3$P - 2s $2p^3$ $^3S^o$, $2s^2$ $2p^2$ $^3$P - 2s $2p^3$ $^3P^o$ and $2s^2$ $2p^2$ $^3$P - 2s $2p^3$ $^3D^o$ were computed using the CW code adapted by Kramida (2018).

Tables from 6 to 8 give the weighted oscillator strengths and transition probability values of these transitions for Ca XV ion obtained *ab initio* by CW code and just compared with Ekman *et al.* (2014) values which are calculated using the MCHF method because there is no data to compare in NIST atomic database (Kramida *et al.*, 2018).

**Table 6.** Weighted oscillator strengths and transition probabilities for the transition ($2s^2 2p^2$ $^3$P - 2s $2p^3$ $^3S^o$) of Ca XV ion. $\log gf$(CW), $\log gf$(EK) and $gA$(CW) and $gA$(EK) are the weighted oscillator strengths and transition probabilities calculated by us and by Ekman *et al.* using the Cowan and (MCDHF) respectively. $g_i$ and $g_k$ are respectively the statistical wights of the term $^3$P -$^3S^o$.

| | | | $\log gf$ | | $gA$ | |
|---|---|---|---|---|---|---|
| $\lambda$ (nm) | $g_i$ | $g_k$ | (CW) | (EK) | (CW) | (EK) |
| 13.9 | 5 | 3 | -0.317 | -0.462 | 1.68E+11 | 1.11E+11 |
| 13.5 | 3 | 3 | -0.599 | -0.762 | 9.22E+10 | 5.82E+10 |
| 13.2 | 1 | 3 | -1.076 | -1.249 | 3.21E+10 | 2.00E+10 |

So, for the results of weighted oscillator strengths $\log gf$ for selected transitions, we found that our results for $2s^2$ $2p^2$ $^3$P - 2s $2p^3$ $^3P^o$ transitions were in a good agreement (the difference is 3.6% for $\log gf$) with the values of Ekman *et al.* Also, for the other transitions, the results differ from the Ekman *et al.* values by about 20% for $2s^2 2p^2$ $^3$P - 2s $2p^3$ $^3S^o$ and 17% for $2s^2 2p^2$ $^3$P - 2s $2p^3$ $^3D^o$.

On the other hand, the results for transition probabilities $gA$ for selected transitions were compared to the values of the Ekman *et al.*: The CW calculated

**Table 7.** Same as Table 6, but for the transition ($2s^2 2p^2\ ^3P$ - $2s\ 2p^3\ ^3P^o$) of Ca XV.

| | | | $\log gf$ | | $gA$ | |
|---|---|---|---|---|---|---|
| $\lambda$ (nm) | $g_i$ | $g_k$ | (CW) | (EK) | (CW) | (EK) |
| 17.46058 | 5 | 3 | -1.34 | -1.32 | 1.01E+10 | 9.54E+09 |
| 17.36467 | 5 | 5 | -0.59 | -0.61 | 5.75E+10 | 4.91E+10 |
| 16.95419 | 3 | 1 | -1.25 | -1.25 | 1.31E+10 | 1.20E+10 |
| 16.90512 | 3 | 3 | -1.07 | -1.12 | 1.98E+10 | 1.61E+10 |
| 16.8152 | 3 | 5 | -1.68 | -1.54 | 4.94E+09 | 6.15E+09 |
| 16.45036 | 1 | 3 | -1.41 | -1.37 | 9.59E+09 | 9.66E+09 |

**Table 8.** Same as Table 6, but for the transition ($2s^2 2p^2\ ^3P$ - $2s\ 2p^3\ ^3D^o$) of Ca XV.

| | | | $\log gf$ | | $gA$ | |
|---|---|---|---|---|---|---|
| $\lambda$ (nm) | $g_i$ | $g_k$ | (CW) | (EK) | (CW) | (EK) |
| 20.25 | 5 | 5 | -1.790 | -2.105 | 2.64E+09 | 1.11E+09 |
| 20.22 | 5 | 3 | -2.992 | -3.365 | 1.66E+08 | 6.15E+07 |
| 20.05 | 5 | 7 | -0.500 | -0.699 | 5.24E+10 | 2.88E+10 |
| 19.51 | 3 | 5 | -0.644 | -0.815 | 3.98E+10 | 2.34E+10 |
| 19.48 | 3 | 3 | -1.399 | -1.616 | 7.02E+09 | 3.72E+09 |
| 18.88 | 1 | 3 | -0.956 | -1.126 | 2.07E+10 | 1.24E+10 |

data for $2s^2\ 2p^2\ ^3P$ - $2s\ 2p^3\ ^3P^o$ transition was in average less than 13% higher of the Ekman *et al.* values, but for $2s^2\ 2p^2\ ^3P$ - $2s\ 2p^3\ ^3S^o$ transition was in average 57% higher of the Ekman *et al.* values and for $2s^2\ 2p^2\ ^3P$ - $2s\ 2p^3\ ^3D^o$ transition the difference reach 100%.

## 4. Conclusion

When comparing the calculated energy levels with experimental values from NIST and the results from Ekman *et al.*, we find that our results for configurations $2s^2\ 2p2$, $2s\ 2p^3$ and $2s^2\ 2p\ 3d$ were close to the NIST database by about 4% to 9%. While, for the other configurations, there are no values to compare with them in NIST, but we found values in the Ekman *et al.* for these configurations except the $2s^2\ 2p\ 5s$ configuration. So, we got new values with the CW code for the ($2s^2\ 2p\ 5s$) configuration and for the term ($2s^2\ 2p\ 4p\ ^1S$) that did not exist before in any experimental data.

As for the results obtained with CW code for all the above transitions of weighted oscillator strengths $\log gf$ are in a good agreement with the values of Ekman *et al.* Also, the results of transition probabilities $gA$ for selected transitions are close to Ekman *et al.* values. For example, the weighted oscillator

strengths and transition probabilities for $2s^2 2p^2\ ^3P$ - $2s\ 2p^3\ ^3P^o$ transitions are in average 3.6% for $\log gf$ and 12% for $gA$ different from the values of Ekman *et al.*

As we mentioned before, there is no abundant data for Ca XV transitions in NIST database, where there are only 14 lines for it (Kramida *et al.*, 2018). So, this study is extremely important to overcome this great lack on atomic structure data for Ca XV ion and it provides the missing values of NIST database and supports the results given by Ekman *et al.* for the weighted oscillator strengths $gf$ and transition probabilities $gA$ which will be very important for the atomic data needed in astrophysical spectroscopy and laboratories.

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