

Atomic structure of the carbon like ion Ca XV

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- **Introduction (Ca XV ion)**
- The Hartree-Fock Relativistic (HFR) theory

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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.

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We can obtain ionized calcium by many approaches, for example, Tokamaks or the solar flare plasma which contain Extreme Ultra-Violet (XUV) solar emission lines of highly ionized calcium.

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In quantum physics the basic equation to be solved is the Schrödinger equation:

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

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The N-electron wavefunction used is the Slater Determinant:

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

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The Hartree-Fock Relativistic (HFR) theory

12th SCSSLA
3-7. June 2019
Vrdnik, Serbia

6

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We used the first eight configurations of Ca XV:

$2s^2 2p^2$

$2s^2 2p 3p$

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$2s 2p^3$

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$2s^2 2p 4s$

$2s^2 2p 5s$

$2s^2 2p 3d$

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as input of the Cowan atomic structure code (2018).

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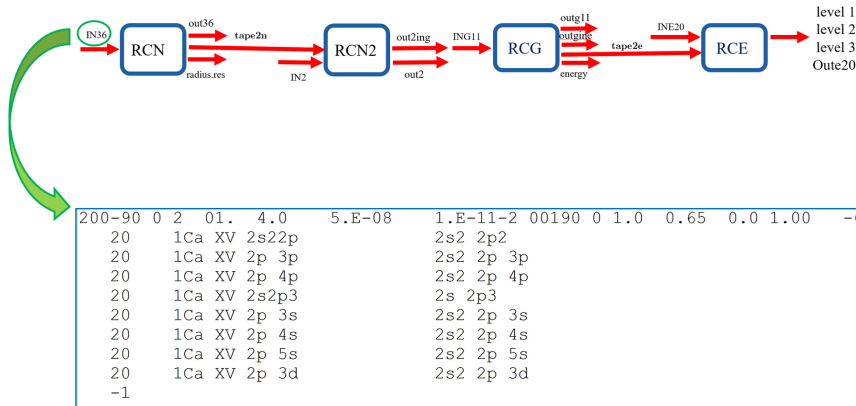
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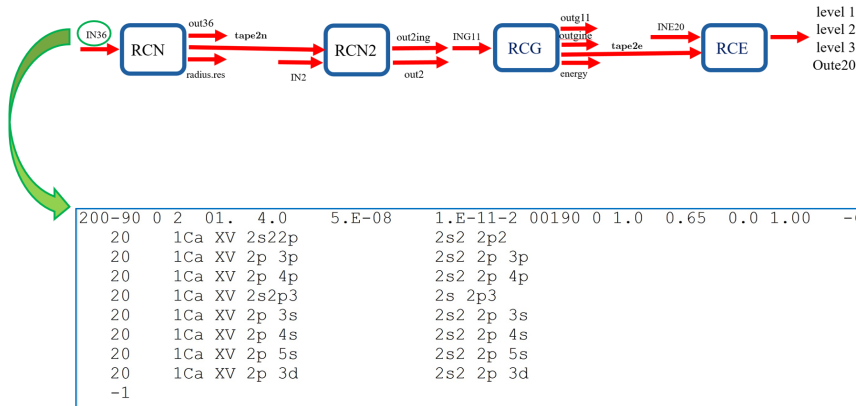
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12th SC SLISA
3-7. June 2019
Vrdnik, Serbia

8




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12th SCSLSA
3-7. June 2019
Vrdnik, Serbia

9

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1 G5INP 0 10 0 0.00002      0011111 1 00000000 9499949494 5.00 1 07200 0.0  
2 -1
```



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12th SCSSLA
3-7. June 2019
Vrdnik, Serbia

9

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The Slater scalings for highly ionized

94% | 99% | 94% | 94% | 94%

F^K the radial integration between equivalent electrons

ξ_{nl} the Spin-orbit parameters

F^K the radial integration between nonequivalent electrons

G^K the exchange integral between nonequivalent electrons

R^K the radial configuration interaction integrals

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12th SCSSLA
3-7. June 2019
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All these ratios are normally used for reasonably good ab initio predictions when using Cowan's Code.

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12th SCSSLA
3-7. June 2019
Vrdnik, Serbia

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Atomic structure of the Ca XV ion

1. Energy levels of the Ca XV:

"Energy levels for the configuration $2s^2 2p^2$ of Ca XV."

$E(\text{NIST})$ are from NIST database, $E(\text{CW})$ are the energy levels calculated by using the Cowan (CW) code, and $E(\text{EK})$ calculated by Ekman et al. using the MCDHF method. All energies are in cm^{-1} .

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$2s^2 2p^2$	$3P$	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
				4.3%	0.1%

-Ekman et al. (2014), *Astronomy and Astrophysics*, **564**, A24.

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$2s^2 2p3s$	$3p^o$	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
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$2s^2 2p4s$	$1p^o$	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	-

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$2s^2 2p3p$	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
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$2s^2 2p3p$	1D	2	-	4528268	4314496
$2s^2 2p3p$	1S	0	-	4567681	4361378

"Energy levels for the configuration $2s^2 2p 4p$ 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 by Ekman et al. using the MCDHF method. All energies are in cm^{-1} .

Conf.	Term	J	E(NIST)	E(CW)	E(EK)
$2s^2 2p4p$	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
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Atomic structure of the Ca XV ion

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

9.6% 0.03%

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9.6% **0.03%**

2. Oscillator strengths and transition probabilities of the different transitions for Ca XV:

"Weighted oscillator strengths and transition probabilities for the transition ($2s^2 2p^2 \ ^3P - 2s \ 2p^3 \ ^3S^o$) 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 code and the MCDHF method respectively. g_i and g_k are respectively the statistical weights of the term $^3P - ^3S^o$.

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λ (nm)	g_i	g_k	$\log gf$		gA	
			(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
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λ (nm)	g_i	g_k	$\log gf$		gA	
			(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
			3.6%		12.6%	

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λ (nm)	g_i	g_k	$\log gf$		gA	
			(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
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