

# The fully relativistic multi-configuration Dirac-Hartree-Fock method for atomic structure calculations for multiply charged ions: The example of Ca XV

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# OUTLINE

- ▶ The Multi-Configuration Dirac-Hartree-Fock (MCDHF) method
- ▶ The GRASP atomic structure code
- ▶ Atomic structure of the Ca XV ion:
  - Energy levels
  - Oscillator strengths and transition probabilities
- ▶ Conclusions and perspectives

In quantum physics the basic equation to be solved is

### “Schrödinger equation”

$$H\Psi(q_1, q_2, \dots, q_N) = E\Psi(q_1, q_2, \dots, q_N)$$

Exact solution for the hydrogen atom (in CQ and RQ mechanics)

**BUT !!**

In the case of atoms consisting of two or more electrons, we cannot solve exactly this equation,  
so we used some approximate methods like

The Hartree–Fock Pseudo–Relativistic  
method with Breit–Pauli corrections

**(HFR + BP)**

(By using Cowan2018 code)

The multiconfiguration Dirac–Hartree–Fock  
method with Breit and QED corrections

**(MCDHF + Breit + QED)**

(By using GRASP2018 code)

## The Multiconfiguration Dirac-Hartree-Fock (MCDHF) method

All the atomic calculations are based on a Hamiltonian. So, we will start with the  
**“Dirac–Coulomb Hamiltonian”**

$$H_{DC} = \sum_{i=1}^N \left( c \alpha_i \cdot p_i + (\beta_i - 1)c^2 + V_{nuc}(r_i) \right) + \sum_{i>j} \frac{1}{r_{ij}}$$

The atomic state function (**ASF**) for N-electrons system is generated by a linear combination of appropriate configuration state functions (**CSFs**)

$$\Psi(\gamma PJM_J) = \sum_{j=1}^{N_{CSF}} c_j \Phi(\gamma_j PJM_J)$$

The most important correction is the transverse photon interaction  
**“Breit interaction”**

which must be include in the Hamiltonian

$$H_{Breit} = - \sum_{i<1}^N \left[ \alpha_i \cdot \alpha_j \frac{\cos(\omega_{ij} r_{ij}/c)}{r_{ij}} + (\alpha_i \cdot \nabla)(\alpha_j \cdot \nabla) \frac{\cos(\omega_{ij} r_{ij}/c) - 1}{\omega_{ij}^2 r_{ij}/c^2} \right]$$

## The Multi-Configuration Dirac-Hartree-Fock (MCDHF) method

The Breit interaction leading quantum electrodynamic (**QED**) corrections which can be included in the calculations of the subsequent relativistic configuration interaction (**RCI**)

Finally, GRASP calculations are used to generate an orbital basis which gives the final wave functions which are obtained in RCI calculations based on the frequency dependent

**“Dirac-Coulomb-Breit Hamiltonian”**

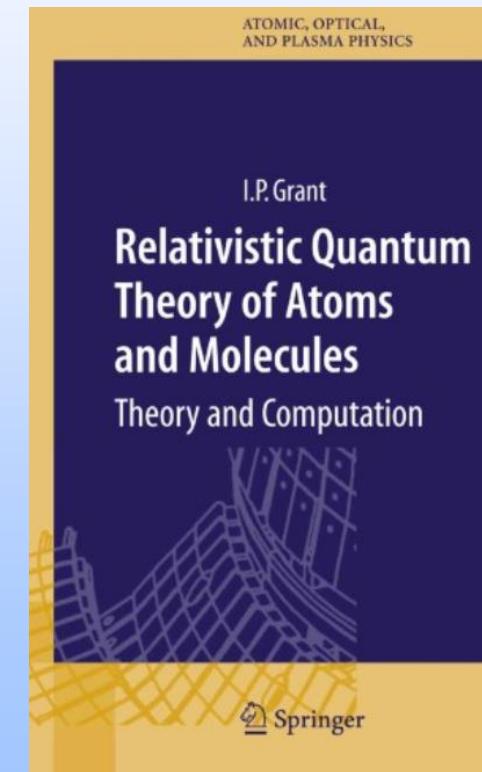
$$H_{DCB} = H_{DC} + H_{Breit}$$

$$H_{DCB} = H_{DC} - \sum_{i < l}^N \left[ \alpha_i \cdot \alpha_j \frac{\cos(\omega_{ij} r_{ij} / c)}{r_{ij}} + (\alpha_i \cdot \nabla)(\alpha_j \cdot \nabla) \frac{\cos(\omega_{ij} r_{ij} / c) - 1}{\omega_{ij}^2 r_{ij} / c^2} \right]$$

# Versions of the GRASP atomic structure code

## GRASP (General Relativistic Atomic Structure Package)

- ▶ GRASP (in 1979)
- ▶ GRASP92 (V1, V2, in F77, 1989)
- ▶ GRASP2K (in F77+COMMONs)
- ▶ GRASP2018 (in F95 +modules +generations of LaTeX tables)
  
- ▶ Grant, I. P. (1979). Relativistic atomic structure calculations. *Computer Physics Communications*, 17(1-2), 149-161.
- ▶ Fischer, C. F., Gaigalas, G., Jönsson, P., & Bieroń, J. (2019). GRASP2018—A Fortran 95 version of the general relativistic atomic structure package. *Computer Physics Communications*, 237, 184-187.

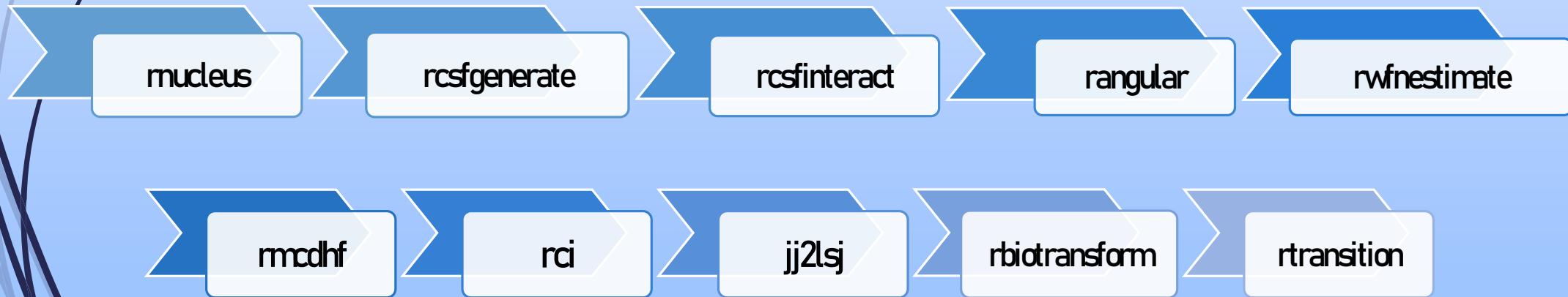


2007

# The GRASP2018 atomic structure code

It is based on the fully relativistic (four-components) multiconfiguration Dirac-Hartree-Fock (MCDHF) method and are suitable for medium to heavy atomic systems.

## Flow of files for a normal sequence of program running in the GRASP2018 code



## “Definition of the most important subroutines in GRASP2018”

8

### **mucleus**

Defines nuclear properties (charge, spin, etc)

### **rcsfgenerate**

Generates the list of CSFs based on rules from wrapper program

### **rcsfinteract**

Removes unimportant CSFs based on analysis of couplings

### **rangular**

Perform angular integration and set up energy expression

### **rwfnestimate**

Initial estimate of radial orbitals

## “Definition of the most important program runs in GRASP2018”

9

**rmcdhf**

Determines both radial orbitals and expansion coefficients

**rci**

Adds transverse Breit and QED corrections and determine only expansion coefficients

**jj2lsj**

Transforms from jj-coupling to LSJ-coupling

**rbiotransform**

Transforms radial orbitals to biorthonormal basis

**rtransition**

Computes transition parameters

## The carbon like ion: Ca XV



### Ca XV ion

Is a highly charged C-like ion that typically exists in high temperature plasma.

There are many approaches to obtain ionized calcium, for example,

- Tokamaks
- The solar flare plasma

The important of Ca XV ion:

- It is interesting for possible astrophysical plasma diagnostic applications.
- It is important for investigation in plasma physics, fusion research and plasma technologies.

# The GRASP2018 atomic structure code



We used the nine  
first  
configurations of  
Ca XV

$2s^2 2p^2$   
 $2s^2 2p 3p$   
 $2s^2 2p 4p$   
 $2s^2 2p 5p$   
 $2s 2p^3$   
 $2s^2 2p 3s$   
 $2s^2 2p 4s$   
 $2s^2 2p 5s$   
 $2s^2 2p 3d$

# The GRASP2018 atomic structure code



## rcsfgenerate

```

*
1
2s(2,i)2p(2,i)
2s(2,i)2p(1,i)3p(1,i)
2s(2,i)2p(1,i)4p(1,i)
2s(2,i)2p(1,i)5p(1,i)

5s,5p,5d,5f,5g
0,6
0
y
2s(2,i)2p(1,i)3s(1,i)
2s(2,i)2p(1,i)4s(1,i)
2s(2,i)2p(1,i)3d(1,i)
2s(2,i)2p(1,i)5s(1,i)
2s(2,i)2p(1,i)4d(1,i)
2s(2,i)2p(1,i)6s(1,i)
2s(2,i)2p(1,i)7s(1,i)
2s(1,i)2p(3,i)

7s,7p,7d,7f,7g,7h
0,8
0
n
  
```

Default, reverse, symmetry or user specified ordering? (\*/r/s/u)

>>

Select core

0: No core

1: He (1s (2) = 2 electrons)

2: Ne ([He] + 2s (2)2p (6) = 10 electrons), etc.

>>

Enter list of (maximum 100) configurations. End list with a blank line or an asterisk (\*)

Give configuration

>>

Give set of active orbitals, as defined by the highest principal quantum number per l-symmetry, in a comma delimited list in s, p, d etc. order,

>>

Resulting 2\*J-number? lower, higher (J=1 -> 2\*J=2 etc.)

>>

Number of excitations

>>

Generate more lists? (y/n)

>>

# Atomic structure of Ca XV ion

## ➤ Energy levels of Ca XV ion

**“Energy levels for the configuration  $2s^2 2p^2$  of Ca XV”**

E(NIST) are from NIST database. E(CW) and E(GRASP) are energy levels calculated by using the Cowan, and GRASP2018 codes, respectively. E(EK) are calculated by Ekman et al. (2014). All energies are in  $cm^{-1}$ .

Conf.	Term	J	E(NIST)	E(CW)	E(GRASP)	E(EK)
$2s^2 2p^2$	$^3P$	0	0	0	0	0
$2s^2 2p^2$	$^3P$	1	17559	16353	17400	17553
$2s^2 2p^2$	$^3P$	2	35923	35171	35749	35920
$2s^2 2p^2$	$^1D$	2	108600	104491	109454	108736
$2s^2 2p^2$	$^1S$	0	197670	214620	199890	197839

**3.8 %      < 1 %      < 1 %**

- Kramida et al. 2018, NIST Atomic Spectra Database (ver. 5.6.1). <https://physics.nist.gov/asd>.
- Alwadie et al. 2020, Contrib. Astron. Obs. Skalnaté Pleso, **50**, 86.
- Ekman et al. 2014, Astronomy and Astrophysics, **564**, A24.

# Atomic structure of Ca XV ion

**“Energy levels for the configuration  $2s\ 2p^3$  of Ca XV”**

E(NIST) are from NIST database. E(CW) and E(GRASP) are energy levels calculated by using the Cowan, and GRASP2018 codes, respectively. E(EK) are calculated by Ekman et al. (2014). All energies are in  $cm^{-1}$ .

Conf.	Term	J	E(NIST)	E(CW)	E(GRASP)	E(EK)
$2s\ 2p^3$	$^5S^o$	2	275900	311928	278840	275788
$2s\ 2p^3$	$^3D^o$	3	500230	533862	492786	500273
$2s\ 2p^3$	$^3D^o$	2	496680	529034	489246	496724
$2s\ 2p^3$	$^3D^o$	1	497570	529652	490283	497632
$2s\ 2p^3$	$^3P^o$	1	582780	607890	574222	582942
$2s\ 2p^3$	$^3P^o$	2	585670	611053	577040	585800
$2s\ 2p^3$	$^3P^o$	0	581730	606177	573031	581886
$2s\ 2p^3$	$^1D^o$	2	729650	759011	737361	730043
$2s\ 2p^3$	$^3S^o$	1	728880	757132	740513	729176
$2s\ 2p^3$	$^1P^o$	1	814380	835599	820709	814815

5.6 %

1.3 %

0.02 %

# Atomic structure of Ca XV ion

**“Energy levels for the configuration  $2s^2\ 2p\ ns\ (n=3,4,5)$  of Ca XV”**

E(NIST) are from NIST database. E(CW) and E(GRASP) are energy levels calculated by using the Cowan, and GRASP2018 codes, respectively. E(EK) are calculated by Ekman et al. (2014). All energies are in  $cm^{-1}$ .

Conf.	Term	J	E(NIST)	E(CW)	E(GRASP)	E(EK)
$2s^2\ 2p\ 3s$	$^3P^o$	0	-	4392032	4092266	4079795
$2s^2\ 2p\ 3s$	$^3P^o$	1	-	4396297	4097178	4084845
$2s^2\ 2p\ 3s$	$^3P^o$	2	-	4428144	4129262	4115926
$2s^2\ 2p\ 3s$	$^1P^o$	1	-	4441352	4146418	4115926
$2s^2\ 2p\ 4s$	$^3P^o$	0	-	4395728	5522657	4115926
$2s^2\ 2p\ 4s$	$^3P^o$	1	-	4396731	5524714	5522133
$2s^2\ 2p\ 4s$	$^3P^o$	2	-	4431652	5559939	5556429
$2s^2\ 2p\ 4s$	$^1P^o$	1	-	4433840	5565137	5561725
$2s^2\ 2p\ 5s$	$^3P^o$	0	-	4657441	6154333	-
$2s^2\ 2p\ 5s$	$^3P^o$	1	-	4657861	6155334	-
$2s^2\ 2p\ 5s$	$^3P^o$	2	-	4693386	6191681	-
$2s^2\ 2p\ 5s$	$^1P^o$	1	-	4694256	6194047	-

# Atomic structure of Ca XV ion

**“Energy levels for the configuration  $2s^2 2p 3p$  of Ca XV”**

E(NIST) are from NIST database. E(CW) and E(GRASP) are energy levels calculated by using the Cowan, and GRASP2018 codes, respectively. E(EK) are calculated by Ekman et al. (2014). All energies are in  $cm^{-1}$ .

Conf.	Term	J	E(NIST)	E(CW)	E(GRASP)	E(EK)
$2s^2 2p 3p$	$^3S$	1	-	4476007	4273284	4257457
$2s^2 2p 3p$	$^1P$	1	-	4446957	4242688	4228086
$2s^2 2p 3p$	$^3D$	1	-	4424400	4218724	4205709
$2s^2 2p 3p$	$^3D$	2	-	4445944	4241564	4229376
$2s^2 2p 3p$	$^3D$	3	-	4472023	4268071	4255295
$2s^2 2p 3p$	$^3P$	0	-	4475994	4273668	4250224
$2s^2 2p 3p$	$^3P$	1	-	4494910	4292428	4270847
$2s^2 2p 3p$	$^3P$	2	-	4501838	4299356	4276163
$2s^2 2p 3p$	$^1D$	2	-	4528268	4327670	4314496
$2s^2 2p 3p$	$^1S$	0	-	4567681	4370566	4361378

# Atomic structure of Ca XV ion

**“Energy levels for the configuration  $2s^2 2p 4p$  of Ca XV”**

E(NIST) are from NIST database. E(CW) and E(GRASP) are energy levels calculated by using the Cowan, and GRASP2018 codes, respectively. E(EK) are calculated by Ekman et al. (2014). All energies are in  $cm^{-1}$ .

Conf.	Term	J	E(NIST)	E(CW)	E(GRASP)	E(EK)
$2s^2 2p 4p$	$^3S$	1	-	4491238	5623387	5618735
$2s^2 2p 4p$	$^1P$	1	-	4487896	5616495	5612050
$2s^2 2p 4p$	$^3D$	1	-	4450829	5575233	5572096
$2s^2 2p 4p$	$^3D$	2	-	4456178	5586794	5583680
$2s^2 2p 4p$	$^3D$	3	-	4488453	5617297	5613455
$2s^2 2p 4p$	$^3P$	0	-	4459660	5594494	5590557
$2s^2 2p 4p$	$^3P$	1	-	4455693	5586486	5582839
$2s^2 2p 4p$	$^3P$	2	-	4491171	5623742	5619232
$2s^2 2p 4p$	$^1D$	2	-	4496043	5635098	5631037
$2s^2 2p 4p$	$^1S$	0	-	4501924	5650682	-

# Atomic structure of Ca XV ion

**“Energy levels for the configuration  $2s^2 2p 5p$  of Ca XV”**

E(NIST) are from NIST database. E(CW) and E(GRASP) are energy levels calculated by using the Cowan, and GRASP2018 codes, respectively. E(EK) are calculated by Ekman et al. (2014). All energies are in  $cm^{-1}$ .

Conf.	Term	J	E(NIST)	E(CW)	E(GRASP)	E(EK)
$2s^2 2p 5p$	$^1P$	1	-	-	6219916	-
$2s^2 2p 5p$	$^3D$	1	-	-	6180901	-
$2s^2 2p 5p$	$^3P$	0	-	-	6190243	-
$2s^2 2p 5p$	$^3P$	1	-	-	6186433	-
$2s^2 2p 5p$	$^1S$	0	-	-	6235500	-

# Atomic structure of Ca XV ion

## “Energy levels for the configuration $2s^2\ 2p\ 3d$ of Ca XV”

E(NIST) are from NIST database. E(CW) and E(GRASP) are energy levels calculated by using the Cowan, and GRASP2018 codes, respectively. E(EK) are calculated by Ekman et al. (2014). All energies are in  $cm^{-1}$ .

Conf.	Term	J	E(NIST)	E(CW)	E(GRASP)	E(EK)
$2s^2\ 2p\ 3d$	$^3F^o$	2	4363300	3951477	4371900	4363635
$2s^2\ 2p\ 3d$	$^3F^o$	3	4379400	3963833	4386983	4378814
$2s^2\ 2p\ 3d$	$^3F^o$	4	-	3988654	4409942	4401309
$2s^2\ 2p\ 3d$	$^3D^o$	2	-	3966033	4394846	4385007
$2s^2\ 2p\ 3d$	$^3D^o$	1	4399500	3975409	4412579	4402470
$2s^2\ 2p\ 3d$	$^3D^o$	2	4411500	3991878	4423464	4413002
$2s^2\ 2p\ 3d$	$^3D^o$	3	4426400	4000316	4436211	4425526
$2s^2\ 2p\ 3d$	$^3P^o$	2	4435400	4006954	4444059	4433389
$2s^2\ 2p\ 3d$	$^3P^o$	1	4434500	4008947	4446056	4435381
$2s^2\ 2p\ 3d$	$^3P^o$	0	-	4010358	4447572	4436968
$2s^2\ 2p\ 3d$	$^1F^o$	3	4475000	4032514	4485377	4474373
$2s^2\ 2p\ 3d$	$^1P^o$	1	4473400	4032524	4484148	4475119

9.7 %      0.2 %      0.03 %

# Atomic structure of Ca XV ion

## ➤ Oscillator strengths and transition probabilities

**“Oscillator strengths of  $2s\ 2p^3 - 2s^2\ 2p^2$  transitions”**

Conf <sub>i</sub>	Term <sub>i</sub>	Conf <sub>k</sub>	Term <sub>k</sub>	g <sub>i</sub>	g <sub>k</sub>	λ (Å)	gf(CW)	gf(GRASP)	gf(EK)
$2s\ 2p^3$	$^3S_1^o$	$2s^2\ 2p^2$	$^3P_2$	5	3	138.9	0.476	0.354	0.345
$2s\ 2p^3$	$^3S_1^o$	$2s^2\ 2p^2$	$^3P_1$	3	3	135.4	0.247	0.180	0.173
$2s\ 2p^3$	$^3S_1^o$	$2s^2\ 2p^2$	$^3P_0$	1	3	132.3	0.083	0.060	0.056
$2s\ 2p^3$	$^3P_2^o$	$2s^2\ 2p^2$	$^3P_1$	5	3	175.2	0.045	0.051	0.048
$2s\ 2p^3$	$^3P_2^o$	$2s^2\ 2p^2$	$^3P_2$	5	5	174.2	0.261	0.246	0.244
$2s\ 2p^3$	$^3P_1^o$	$2s^2\ 2p^2$	$^3P_0$	3	1	170.2	0.056	0.042	0.056
$2s\ 2p^3$	$^3P_1^o$	$2s^2\ 2p^2$	$^3P_1$	3	3	169.7	0.086	0.074	0.076
$2s\ 2p^3$	$^3P_1^o$	$2s^2\ 2p^2$	$^3P_2$	3	5	168.7	0.020	0.028	0.029
$2s\ 2p^3$	$^3P_0^o$	$2s^2\ 2p^2$	$^3P_1$	1	3	165.0	0.038	0.057	0.043
$2s\ 2p^3$	$^3D_2^o$	$2s^2\ 2p^2$	$^3P_2$	5	5	202.1	0.015	0.007	0.008
$2s\ 2p^3$	$^3D_2^o$	$2s^2\ 2p^2$	$^3P_1$	5	3	201.9	0.001	0.000	0.000
$2s\ 2p^3$	$^3D_2^o$	$2s^2\ 2p^2$	$^3P_3$	5	7	200.1	0.315	0.202	0.200
$2s\ 2p^3$	$^3D_1^o$	$2s^2\ 2p^2$	$^3P_2$	3	5	194.8	0.228	0.155	0.153
$2s\ 2p^3$	$^3D_1^o$	$2s^2\ 2p^2$	$^3P_1$	3	3	194.6	0.039	0.024	0.024
$2s\ 2p^3$	$^3D_0^o$	$2s^2\ 2p^2$	$^3P_1$	1	3	188.5	0.112	0.076	0.075

# Atomic structure of Ca XV ion

**“Transition probabilités of  $2s\ 2p^3 - 2s^2\ 2p^2$  transitions”**

Conf <sub>i</sub>	Term <sub>i</sub>	Conf <sub>k</sub>	Term <sub>k</sub>	g <sub>i</sub>	g <sub>k</sub>	λ (Å)	gA(CW)	gA(GRASP)	gA(EK)
$2s\ 2p^3$	$^3S_1^o$	$2s^2\ 2p^2$	$^3P_2$	5	3	138.9	1.616E+11	1.225E+11	1.107E+11
$2s\ 2p^3$	$^3S_1^o$	$2s^2\ 2p^2$	$^3P_1$	3	3	135.4	8.833E+10	6.543E+10	5.820E+10
$2s\ 2p^3$	$^3S_1^o$	$2s^2\ 2p^2$	$^3P_0$	1	3	132.3	3.081E+10	2.280E+10	2.001E+10
$2s\ 2p^3$	$^3P_2^o$	$2s^2\ 2p^2$	$^3P_1$	5	3	175.2	9.759E+09	1.042E+10	9.540E+09
$2s\ 2p^3$	$^3P_2^o$	$2s^2\ 2p^2$	$^3P_2$	5	5	174.2	5.729E+10	5.045E+10	4.910E+10
$2s\ 2p^3$	$^3P_1^o$	$2s^2\ 2p^2$	$^3P_0$	3	1	170.2	1.299E+10	1.235E+10	1.200E+10
$2s\ 2p^3$	$^3P_1^o$	$2s^2\ 2p^2$	$^3P_1$	3	3	169.7	2.002E+10	1.614E+10	1.611E+10
$2s\ 2p^3$	$^3P_1^o$	$2s^2\ 2p^2$	$^3P_2$	3	5	168.7	4.573E+09	6.235E+09	6.150E+09
$2s\ 2p^3$	$^3P_0^o$	$2s^2\ 2p^2$	$^3P_1$	1	3	165.0	9.302E+09	9.618E+09	9.660E+09
$2s\ 2p^3$	$^3D_2^o$	$2s^2\ 2p^2$	$^3P_2$	5	5	202.1	2.456E+09	1.085E+09	1.110E+09
$2s\ 2p^3$	$^3D_2^o$	$2s^2\ 2p^2$	$^3P_1$	5	3	201.9	1.623E+08	5.028E+07	6.150E+07
$2s\ 2p^3$	$^3D_2^o$	$2s^2\ 2p^2$	$^3P_3$	5	7	200.1	5.243E+10	2.999E+10	2.877E+10
$2s\ 2p^3$	$^3D_1^o$	$2s^2\ 2p^2$	$^3P_2$	3	5	194.8	4.014E+10	2.444E+10	2.340E+10
$2s\ 2p^3$	$^3D_1^o$	$2s^2\ 2p^2$	$^3P_1$	3	3	194.6	6.874E+09	3.837E+09	3.720E+09
$2s\ 2p^3$	$^3D_0^o$	$2s^2\ 2p^2$	$^3P_1$	1	3	188.5	2.100E+10	1.288E+10	1.236E+10

55 %      5.7 %

# Atomic structure of Ca XV ion



**“Oscillator strengths of  $2s^2 2p\ ns - 2s^2 2p\ 3p$  transitions”**

Conf <sub>i</sub>	Term <sub>i</sub>	Conf <sub>k</sub>	Term <sub>k</sub>	g <sub>i</sub>	g <sub>k</sub>	$\lambda$ (Å)	gf(CW)	gf(GRASP)	gf(EK)
$2s^2 2p\ 3s$	$^1P_1^o$	$2s^2 2p\ 3p$	$^1D_2$	3	1	551.7	-	0.514	0.493
$2s^2 2p\ 3s$	$^1P_1^o$	$2s^2 2p\ 3p$	$^1S_0$	3	5	446.1	-	0.139	0.135
$2s^2 2p\ 4s$	$^1P_1^o$	$2s^2 2p\ 3p$	$^1D_2$	3	5	80.8	-	0.281	-
$2s^2 2p\ 4s$	$^1P_1^o$	$2s^2 2p\ 3p$	$^1P_1$	3	3	75.6	-	0.040	-
$2s^2 2p\ 4s$	$^1P_1^o$	$2s^2 2p\ 3p$	$^1S_0$	3	1	83.7	-	0.078	-
$2s^2 2p\ 5s$	$^1P_1^o$	$2s^2 2p\ 3p$	$^1D_2$	3	5	53.6	-	0.055	-
$2s^2 2p\ 5s$	$^1P_1^o$	$2s^2 2p\ 3p$	$^1P_1$	3	3	51.2	-	0.008	-
$2s^2 2p\ 5s$	$^1P_1^o$	$2s^2 2p\ 3p$	$^1S_0$	3	1	54.8	-	0.015	-

# Atomic structure of Ca XV ion

“Transition probabilities of  $2s^2 2p\ ns - 2s^2 2p\ 3p$  transitions”

Conf <sub>i</sub>	Term <sub>i</sub>	Conf <sub>k</sub>	Term <sub>k</sub>	g <sub>i</sub>	g <sub>k</sub>	$\lambda$ (Å)	gA(CW)	gA(GRASP)	gA(EK)
$2s^2 2p\ 3s$	$^1P_1^0$	$2s^2 2p\ 3p$	$^1D_2$	3	1	551.7	-	2.254E+09	2.140E+09
$2s^2 2p\ 3s$	$^1P_1^0$	$2s^2 2p\ 3p$	$^1S_0$	3	5	446.1	-	2.336E+10	2.330E+10
$2s^2 2p\ 4s$	$^1P_1^0$	$2s^2 2p\ 3p$	$^1D_2$	3	5	80.8	-	4.781E+11	-
$2s^2 2p\ 4s$	$^1P_1^0$	$2s^2 2p\ 3p$	$^1P_1$	3	3	75.6	-	4.686E+10	-
$2s^2 2p\ 4s$	$^1P_1^0$	$2s^2 2p\ 3p$	$^1S_0$	3	1	83.7	-	2.481E+10	-
$2s^2 2p\ 5s$	$^1P_1^0$	$2s^2 2p\ 3p$	$^1D_2$	3	5	53.6	-	2.142E+11	-
$2s^2 2p\ 5s$	$^1P_1^0$	$2s^2 2p\ 3p$	$^1P_1$	3	3	51.2	-	2.065E+10	-
$2s^2 2p\ 5s$	$^1P_1^0$	$2s^2 2p\ 3p$	$^1S_0$	3	1	54.8	-	1.121E+10	-

## Conclusions and perspectives

1

MCDHF method is a fully quantum methods, HFR or TFDA are pseudo-relativistic methods.

2

GRASP2018 code gives better results than CW or AS or SS codes.

3

New energy levels, oscillator strengths and transition probabilities for Ca XV are obtained.

4

It's interesting to use the MCDHF code for SCP Stark width calculations.

5

It's interesting to use the MCDHF and DARC codes for Stark width calculations.

**Thank you for your attention**