# SYSTEMATIC ATOMIC STRUCTURE OF THE NEUTRAL COBALT ATOM (Co I)

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# Outline


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- Properties of Co I
- The emission spectrum of Cobalt
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  - TFDA theory
- Atomic structure codes
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- Conclusions


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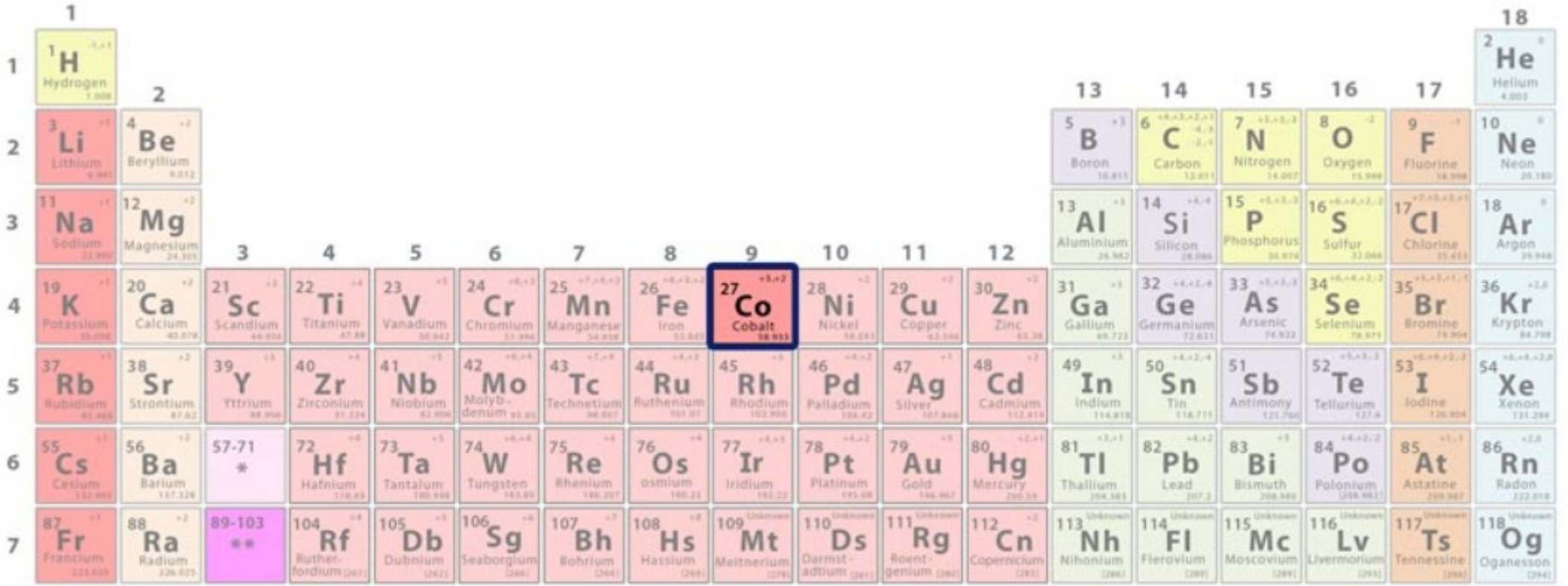
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1 H Hydrogen
2 He Helium
3 Li Lithium
4 Be Beryllium
5 B Boron
6 C Carbon
7 N Nitrogen
8 O Oxygen
9 F Fluorine
10 Ne Neon
11 Na Sodium
12 Mg Magnesium
13 Al Aluminium
14 Si Silicon
15 P Phosphorus
16 S Sulfur
17 Cl Chlorine
18 Ar Argon
19 K Potassium
20 Ca Calcium
21 Sc Scandium
22 Ti Titanium
23 V Vanadium
24 Cr Chromium
25 Mn Manganese
26 Fe Iron
27 Co Cobalt
28 Ni Nickel
29 Cu Copper
30 Zn Zinc
31 Ga Gallium
32 Ge Germanium
33 As Arsenic
34 Se Selenium
35 Br Bromine
36 Kr Krypton
37 Rb Rubidium
38 Sr Strontium
39 Y Yttrium
40 Zr Zirconium
41 Nb Niobium
42 Mo Molyb-denum
43 Tc Technetium
44 Ru Ruthenium
45 Rh Rhodium
46 Pd Palladium
47 Ag Silver
48 Cd Cadmium
49 In Indium
50 Sn Tin
51 Sb Antimony
52 Te Tellurium
53 I Iodine
54 Xe Xenon
55 Cs Cesium
56 Ba Barium
57-71 *
72 Hf Hafnium
73 Ta Tantalum
74 W Tungsten
75 Re Rhenium
76 Os osmium
77 Ir Iridium
78 Pt Platinum
79 Au Gold
80 Hg Mercury
81 Tl Thallium
82 Pb Lead
83 Bi Bismuth
84 Po Polonium
85 At Astatine
86 Rn Radon
87 Fr Francium
88 Ra Radium
89-103 **
104 Rf Ruther-fordium
105 Db Dubnium
106 Sg Seaborgium
107 Bh Bohrium
108 Hs Hassium
109 Mt Meitnerium
110 Ds Darmst-adtium
111 Rg Roent-genium
112 Cn Copernicium
113 Nh Nihonium
114 Fl Flerovium
115 Mc Moscovium
116 Lv Livermorium
117 Ts Tennessine
118 Og Oganesson


## Properties of Co I

Density 8.90 g/cm$^3$

Atomic number: 27

Atomic mass: 58.933195 u

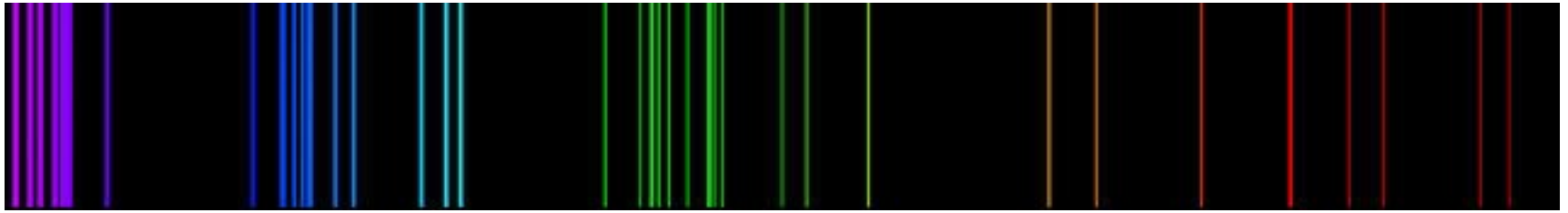
Electronic configuration of Co I: $4s^2\ 3d^7$

Ground-state term of Co I: $^4F_{9/2}$

Ionization energy of Co I: 7.881 eV

Classification: transition metal.

# The emission spectrum of Cobalt




# Theory

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

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

It is possible to obtain exact solutions of this equation only for one-electron systems, i.e., for hydrogen like ions. For many electron systems approximation methods must be used:

1- Hartree-Fock Theory

Obtaining wave functions for the radial equation to get the energy levels.

2- Thomas-Fermi-Dirac-Amaldi Theory (TFDA)

Obtaining effective potentials for the radial equation to get the energy levels.

# 1- H.F Theory


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

Where we used the Slater Determinant as wave function:

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

# 1- H.F Theory


$$\left[-\frac{1}{2}\nabla_{r_i}^2-\frac{Z}{r_i}\right]u_\lambda(q_i)+\left[\sum_\mu \int u_\mu^*(q_i)\frac{1}{r_{ij}}u_\mu(q_j)dq_j\right]u_\lambda(q_i)-\sum_\mu\left[\int u_\mu^*(q_j)\frac{1}{r_{ij}}u_\lambda(q_j)dq_j\right]u_\lambda(q_i)=E_\lambda u_\lambda(q_i) \quad ;\lambda,\mu=\alpha,\beta,\ldots,\nu$$

The solution of this equation is:

$$E[\Psi]=\sum_\lambda I_\lambda+\frac{1}{2}\sum_\lambda\sum_\mu[J_{\lambda\mu}-K_{\lambda\mu}]$$ Where

$$I_\lambda=\left\langle u_\lambda(q_i)\left|\hat{h}_i\right|u_\lambda(q_i)\right\rangle \qquad J_{\lambda\mu}=\left\langle u_\lambda(q_i)u_\mu(q_j)\left|\frac{1}{r_{ij}}\right|u_\lambda(q_i)u_\mu(q_j)\right\rangle \qquad K_{\lambda\mu}=\left\langle u_\lambda(q_i)u_\mu(q_j)\left|\frac{1}{r_{ij}}\right|u_\mu(q_i)u_\lambda(q_j)\right\rangle$$

Where $h_i=-\frac{1}{2}\nabla_{r_i}^2-\frac{Z}{r_i}$

# 2- T.F.D.A Theory


the *Thomas–Fermi–Dirac–Amaldi* (TFDA) model, where the charge distribution is assumed to be spherically symmetric, is a useful procedure to choose the central potential *U(r )*.

the TFDA model gives a

$$U(r) = \frac{\mathcal{Z}_{\text{eff}}(\lambda_{nl}, r)}{r} = -\frac{Z}{r}\phi(x)$$

Where,

$$\phi(x) = e^{-Zr/2} + \lambda_{nl}(1 - e^{-Zr/2}), \quad x = \frac{r}{\mu},$$

and $\mu$ is the constant

Having determined a central potential *U(r )*, we compute the one-electron orbitals $P_{nl}(r)$ by solving the wave equation

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + 2U(r) + \epsilon_{nl}\right] P_{nl}(r) = 0.$$

# 2- T.F.D.A Theory


$$\left[ -\frac{d^2}{dr^2} + \frac{l_i(l_i+1)}{r^2} + V(\lambda,r) \right] P_i(r) = \varepsilon_i P_i(r)$$

Where

$$V(\lambda,r) = \frac{Z_{eff}(\lambda,r)}{r} = -\frac{Z}{r}\phi(x)$$

Where

$$\phi(x) = e^{-\frac{Z}{r}} + \lambda\left(1 - e^{-\frac{Z}{r}}\right), x = \frac{r}{\mu}$$

and $\mu$ is the constant

$$\mu = 0.8853\left(\frac{N-1}{N}\right)^{\frac{2}{3}} Z^{-\frac{1}{3}}$$


# Atomic Structure Codes

- Theoretical atomic data are important for many physics research fields including plasma modeling under various physical conditions, X-ray spectroscopy and astrophysical research.

- Scientists have developed several computer programs that perform atomic calculations.

# Some Atomic Structure Codes


| Code | Author | Method |
|---|---|---|
| Cowan | R. Cowan (1981) | Breit-Pauli, HF method |
| SUPERSTRUCTURE | W. Eissner *et al*. (1974) | Breit-Pauli, TFDA potential |
| AUTOSTRUCTURE | N. R. Badnell (1986) | Breit-Pauli, TFDA potential |
| CIV3 | A. Hibbert (1975) | Non relativistic CI method |
| FAC | M. F. Gu (2008) | MCDF, Breit-Pauli and QED |
| GRASP | F. Parpia and I. Grant (1989) | MCDF or parametric potential. |
| MCHF | C. F.  Fischer (2000) | Non relativistic MCHF approach |

# Configurations used in the atomic structure calculations for Co I


- $3d^7\,4s^2$
- $3d^7\,4s\,4d$
- $3d^7\,4s\,5s$
- $3d^8\,4s$
- $3d^8\,5s$
- $3d^8\,4d$
- $3d^9$
- $3d^7\,4s\,4p$
- $3d^7\,4s\,4f$
- $3d^8 4p$
- $3d^8\,4f$

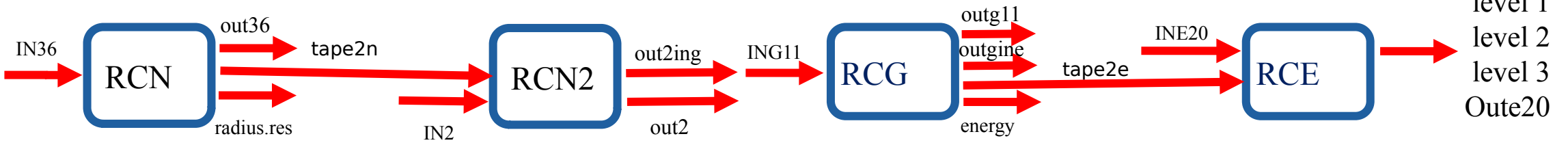
**Atomic structure codes used:**

1- Cowan code developed by R. Cowan (1981).

2- AUTOSTRUCTURE code developed by N. R. Badnell (1986).

[T1]


# Cowan suite of atomic structure codes (CW)



# Cowan suite of atomic structure codes (CW)

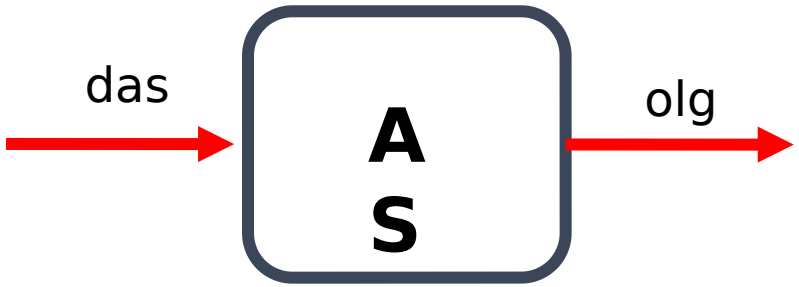

```
200-90 0 2  01.   0.2     5.E-08     1.E-11-2 00190 0 1.0  0.65  0.0 1.00   -6
   27     1Co I  3d74s2          3d7  4s2
   27     1Co I  4s4d            3d7  4s   4d
   27     1Co I  4s5s            3d7  4s   5s
   27     1Co I  3d84s           3d8  4s
   27     1Co I  3d85s           3d8  5s
   27     1Co I  3d84d           3d8  4d
   27     1Co I  3d9             3d9
   27     1Co I  4s4p            3d7  4s   4p
   27     1Co I  4s4f            3d7  4s   4f
   27     1Co I  3d84p           3d8  4p
   27     1Co I  3d84f           3d8  4f
   -1
```

Input file: IN36

# AUTOSTRUCTURE code (AS)


```
A.S.   Co I
 &SALGEB RUN='   ' RAD='E1' CUP='IC'
      MXVORB=6 MXCONF=11 KCOR1=1 KCOR2=5 kutss=-9 kutoo=1 kutso=0 kutssx=-9 kutoox=-1 &END
 3 2 4 0 4 1 4 2 4 3 5 0
 7   2   0   0   0   0
 7   1   1   0   0   0
 7   1   0   1   0   0
 7   1   0   0   1   0
 7   1   0   0   0   1
 8   1   0   0   0   0
 8   0   1   0   0   0
 8   0   0   1   0   0
 8   0   0   0   1   0
 8   0   0   0   0   1
 9   0   0   0   0   0
&SMINIM NZION=27 INCLUD=0 NLAM=11 ISHFTIC=0 QED=0 &END
1.43314  1.13940  1.08274  1.06269  1.04441
1.02479  0.99491  0.96411  0.99683  0.97323
0.95802
1   2   3   4   5   6   7   8   9  10  11
```

Input file: das



# Results of Ab initio Energy Levels ($cm^{-1}$)

| Configuration | Term | J | E(NIST) | E(AS) | E(CW) |
|---|---|---|---|---|---|
| $3p^6 3d^7 4s^2$ | a $^4$F | $^9/_2$ | 0.0 | 0.0 | 0.0 |
| $3p^6 3d^7 4s^2$ | a $^4$F | $^7/_2$ | 816.0 | 817.0 | 812.9 |
| $3p^6 3d^7 4s^2$ | a $^4$F | $^5/_2$ | 1406.8 | 1417.0 | 1406.2 |
| $3p^6 3d^7 4s^2$ | a $^4$F | $^3/_2$ | 1809.3 | 1830.0 | 1811.4 |
| $3p^6 3d^7 4s^2$ | a $^4$P | $^5/_2$ | 13795.5 | 18958.0 | 15149.4 |
| $3p^6 3d^7 4s^2$ | a $^4$P | $^3/_2$ | 14036.3 | 19238.0 | 15384.1 |
| $3p^6 3d^7 4s^2$ | a $^4$P | $^1/_2$ | 14399.3 | 19580.0 | 15790.4 |
| $3p^6 3d^7 4s^2$ | a $^2$G | $^9/_2$ | 16467.9 | 19103.0 | 15085.5 |
| $3p^6 3d^7 4s^2$ | a $^2$G | $^7/_2$ | 17233.7 | 19864.0 | 15867.0 |
| $3p^6 3d^7 4s^2$ | b $^2$P | $^3/_2$ | 20500.7 | 25147.0 | 19554.0 |
| $3p^6 3d^7 4s^2$ | b $^2$P | $^1/_2$ | 21215.9 | 25900.0 | 20380.0 |
| $3p^6 3d^7 4s^2$ | a $^2$H | $^{11}/_2$ | 21780.5 | 25398.0 | 20135.2 |
| $3p^6 3d^7 4s^2$ | b $^2$D | $^5/_2$ | 21920.1 | 27399.0 | 21197.8 |
| $3p^6 3d^7 4s^2$ | a $^2$H | $^9/_2$ | 22475.4 | 26085.0 | 20835.5 |

**18.0 %5.4 %**

# Results of Fitting Energy Levels ($cm^{-1}$)


| Configuration | Term | J | E(NIST) | E_fit(AS) | E_fit(CW) |
|---|---|---|---|---|---|
| $3p^6 3d^7 4s^2$ | a $^4$F | $^9/_2$ | 0.0 | 0.0 | 0.0 |
| $3p^6 3d^7 4s^2$ | a $^4$F | $^7/_2$ | 816.0 | 820.0 | 720.0 |
| $3p^6 3d^7 4s^2$ | a $^4$F | $^5/_2$ | 1406.8 | 1408.0 | 1379.4 |
| $3p^6 3d^7 4s^2$ | a $^4$F | $^3/_2$ | 1809.3 | 1807.0 | 1829.9 |
| $3p^6 3d^7 4s^2$ | a $^4$P | $^5/_2$ | 13795.5 | 13865.0 | 13779.0 |
| $3p^6 3d^7 4s^2$ | a $^4$P | $^3/_2$ | 14036.3 | 14119.0 | 14103.9 |
| $3p^6 3d^7 4s^2$ | a $^4$P | $^1/_2$ | 14399.3 | 14473.0 | 14510.6 |
| $3p^6 3d^7 4s^2$ | a $^2$G | $^9/_2$ | 16467.9 | 16492.0 | 16578.6 |
| $3p^6 3d^7 4s^2$ | a $^2$G | $^7/_2$ | 17233.7 | 17270.0 | 17468.4 |
| $3p^6 3d^7 4s^2$ | b $^2$P | $^3/_2$ | 20500.7 | 20593.0 | 20570.0 |
| $3p^6 3d^7 4s^2$ | b $^2$P | $^1/_2$ | 21215.9 | 21273.0 | 21254.2 |
| $3p^6 3d^7 4s^2$ | a $^2$H | $^{11}/_2$ | 21780.5 | 21825.0 | 21479.8 |
| $3p^6 3d^7 4s^2$ | b $^2$D | $^5/_2$ | 21920.1 | 23104.0 | 22057.4 |
| $3p^6 3d^7 4s^2$ | a $^2$H | $^9/_2$ | 22475.4 | 22534.0 | 25263.6 |

**0.7%** **2.6%**


# Ab initio and fitting calculations

| | CW | AS |
|---|---|---|
| Ab initio calculations | 18.0 % | 5.4 % |
| Fitting calculations | 0.7% | 2.6 % |


# Transition calculations

These calculations are in progress...

# Conclusions


- Ab initio atomic structure calculations (purely theoretical calculations) are done using the CW & AS codes.
- Fitting atomic structure calculations (semi-empirical calculations) are done using the CW & AS codes.
- New data for plasma spectroscopy and astrophysical applications will be provided.


# Thank you

*A. Siddig*