

# Kvantfysik Lecture Notes No. 17

**PERIODIC TABLE**

## Atomic Properties of the Elements

**NIST National Institutes of Standards and Technology**  
Technology Administration, U.S. Department of Commerce

**Physics Laboratory**  
physics.nist.gov

**Standard Reference Data Group**  
www.nist.gov/srd

18 VIIIA  
**He**  
Helium  
2.00385(4)  
4.002602

10  
**Ne**  
Neon  
18.9984032(5)  
20.1797(6)  
36.96515(8)  
79.904(2)  
131.904(4)  
201.968662(9)  
24.3874

17 VIIA  
**F**  
Fluorine  
18.9984032(5)  
19.000  
35.453(2)  
69.723(1)  
17.4228

16 VIA  
**O**  
Oxygen  
15.99903199(6)  
15.999  
32.007(1)  
13.8181

15 VA  
**N**  
Nitrogen  
14.003074004(8)  
14.003  
30.973761(7)  
14.5341

14 IVA  
**C**  
Carbon  
12.010738(8)  
12.011  
12.0107(1)  
11.2603

13 IIIA  
**B**  
Boron  
10.811(3)  
10.811  
10.811(3)

12 IIB  
**Be**  
Beryllium  
9.012182(2)  
9.012  
9.012182(2)

11 IB  
**Li**  
Lithium  
6.941(1)  
6.941  
6.941(1)

10 VIII  
**Na**  
Sodium  
22.98976928(2)  
22.98976928(2)

9 VIII  
**Mg**  
Magnesium  
24.304(6)  
24.304(6)

8 VIII  
**Al**  
Aluminum  
26.9815385(8)  
26.9815385(8)

7 VIIA  
**Si**  
Silicon  
28.0855(8)  
28.0855(8)

6 VIA  
**P**  
Phosphorus  
30.973761(7)  
30.973761(7)

5 VA  
**S**  
Sulfur  
32.06(5)  
32.06(5)

4 IVA  
**Cl**  
Chlorine  
35.453(2)  
35.453(2)

3 IIIA  
**Ar**  
Argon  
39.948(4)  
39.948(4)

2 IIA  
**Ca**  
Calcium  
40.078(4)  
40.078(4)

1 IA  
**H**  
Hydrogen  
1.00784(7)  
1.00784(7)

**Frequently used fundamental physical constants**  
For the most accurate values of these and other constants, visit [physics.nist.gov/constants](http://physics.nist.gov/constants)

1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of <sup>133</sup>Cs  
( $\hbar = h/2\pi$ )

Speed of light in vacuum  $c$  299 792 458 m s<sup>-1</sup> (exact)

Planck constant  $h$  6.626 070 15 × 10<sup>-34</sup> J s (exact)

elementary charge  $e$  1.602 176 634 × 10<sup>-19</sup> C

electron mass  $m_e$  9.109 383 56 × 10<sup>-31</sup> kg

proton mass  $m_p$  1.672 621 637 × 10<sup>-27</sup> kg

fine-structure constant  $\alpha$  1/137.036

Rydberg constant  $R_\infty$  10 973 732 m<sup>-1</sup>

$R_\infty hc$  3.289 842 × 10<sup>15</sup> Hz

$R_\infty hc$  13.6057 eV

Boltzmann constant  $k$  1.380 7 × 10<sup>-23</sup> J K<sup>-1</sup>

**Legend:**  
  Solids  
  Liquids  
  Gases  
  Artificially Prepared

Group	1	2	3	4	5	6	7	8	9	10	11	12
Period	IA	IIA	IIIB	IVB	VB	VIB	VII B	VIII	IX	X	XI	XII
1	<b>H</b> Hydrogen 1.00784(7)	<b>Li</b> Lithium 6.941(1)	<b>Na</b> Sodium 22.98976928(2)	<b>K</b> Potassium 39.0983(1)	<b>Rb</b> Rubidium 85.4678(3)	<b>Cs</b> Cesium 132.90545(2)	<b>Ba</b> Barium 137.327(8)	<b>La</b> Lanthanum 138.905(5)	<b>Ce</b> Cerium 140.116(7)	<b>Pr</b> Praseodymium 140.90765(7)	<b>Nd</b> Neodymium 144.24(2)	<b>Pm</b> Promethium (145)
2	<b>He</b> Helium 4.002602	<b>Be</b> Beryllium 9.012182(2)	<b>Mg</b> Magnesium 24.304(6)	<b>Ca</b> Calcium 40.078(4)	<b>Sr</b> Strontium 87.62(1)	<b>Zr</b> Zirconium 91.224(8)	<b>Nb</b> Niobium 92.90638(2)	<b>Mo</b> Molybdenum 95.94(1)	<b>Tc</b> Technetium (98)	<b>Ru</b> Ruthenium 101.07(2)	<b>Rh</b> Rhodium 102.90550(5)	<b>Pd</b> Palladium 106.42(1)
3	<b>Li</b> Lithium 6.941(1)	<b>Be</b> Beryllium 9.012182(2)	<b>B</b> Boron 10.811(3)	<b>C</b> Carbon 12.0107(1)	<b>N</b> Nitrogen 14.00307(1)	<b>O</b> Oxygen 15.999(1)	<b>F</b> Fluorine 18.998(1)	<b>Ne</b> Neon 20.1797(6)	<b>Na</b> Sodium 22.98976928(2)	<b>Mg</b> Magnesium 24.304(6)	<b>Al</b> Aluminum 26.9815385(8)	<b>Si</b> Silicon 28.0855(8)
4	<b>Li</b> Lithium 6.941(1)	<b>Be</b> Beryllium 9.012182(2)	<b>B</b> Boron 10.811(3)	<b>C</b> Carbon 12.0107(1)	<b>N</b> Nitrogen 14.00307(1)	<b>O</b> Oxygen 15.999(1)	<b>F</b> Fluorine 18.998(1)	<b>Ne</b> Neon 20.1797(6)	<b>Na</b> Sodium 22.98976928(2)	<b>Mg</b> Magnesium 24.304(6)	<b>Al</b> Aluminum 26.9815385(8)	<b>Si</b> Silicon 28.0855(8)
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**Lanthanides**

**Actinides**

**Ground-state Level**

**Symbol** **Ce** <sup>G<sub>4</sub></sup>

**Name** Cerium

**Atomic Weight** 140.116

**Ground-state Configuration** [Xe]4f5d6s<sup>2</sup>

**Ionization Energy (eV)** 5.5387

Based upon <sup>133</sup>C. ( ) indicates the mass number of the most stable isotope. For a description of the data, visit [physics.nist.gov/data](http://physics.nist.gov/data)

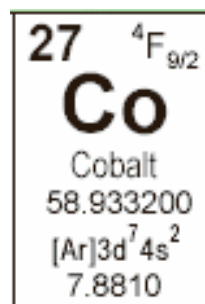
NIST SP 966 (September 2003)

# 1 The periodic table

We now turn to atoms where there are more than one electron. The electrons are identical fermions and we will thus apply our discussions in the lecture 14 notes to this situation. The periodic table is determined by how the electrons of the atom fill up the available shells, starting with the lowest energy levels first. At the most naive level, one ignores the interactions between the electrons, but we will see that the electron interactions play an important role in the structure of the table.

The figure on the previous page shows an especially detailed periodic table from the United States National Institute of Standards (NIST). Of course each square corresponds to an element in nature, with the elements ordered by how many electrons are in the neutral atoms. This particular table actually provides a lot of information for each element, so let us take a moment to review what information is provided in each square.

To the right is the box for Cobalt (**Co**). The number in the upper left corner (27) is the atomic number, which gives the number of protons in the nucleus which is the same as the number of electrons since the atom is neutral. The number underneath “Cobalt” (58.933200) is the atomic weight. The atomic weight is the average mass of the atom in units of 1/12 the mass of a  $^{12}\text{C}$  atom (called atomic mass units). Given this information, you might be wondering why the atomic weight for carbon on the table is 12.01 and not just 12. This is because the elements can appear as various isotopes with different numbers of neutrons in the nucleus. In the case of carbon, there are two stable isotopes,  $^{12}\text{C}$  (“carbon 12”) and  $^{13}\text{C}$  (“carbon 13”), where the 12 and 13 refer to the total number of protons plus neutrons in the nucleus. About 99% of the carbon found in nature is  $^{12}\text{C}$  and the other 1% is  $^{13}\text{C}$ . Since a neutron has almost the same mass as a proton, we would therefore expect carbon’s atomic weight to be shifted up by about 0.01 atomic mass units.



The last number at the bottom of the square (7.8810) is the ionization energy for the atom in units of electron volts (eV). The ionization energy is the energy required to remove one electron from an atom in its ground state. Notice that the ionization energies more or less increase as one moves from

left to right across the table. The elements on the far right are called the noble gases and are chemically the most stable elements. This is because their electrons are most tightly bound to their nuclei, and yet an additional electron would be much less tightly bound.

There are two more pieces of information in the **Co** box, but before explaining what these are let us review the spectroscopic notation. Historically, the various values of orbital angular momentum  $\ell$  are assigned letters. As in the previous lecture we use lower case letters for the orbital angular momentum of individual electrons, with **s**, **p**, **d**, **f**, **g** assigned to  $\ell = 0, 1, 2, 3, 4$  respectively. We use capital letters for the *total* orbital angular momentum of *all* the electrons, with **S**, **P**, **D**, **F**, **G**, **H** . . . assigned to total orbital momentum  $L = 0, 1, 2, 3, 4, 5, 6 \dots$  respectively. (In the hydrogenic case, since there is only one electron its orbital value *is* the total orbital value). The electrons will also have a total spin  $S$  with the total number of spin states given by  $2S + 1$ . Finally the electrons will have a total angular momentum  $J$ . These three quantities are then written together as  $^{2S+1}\mathbf{L}_J$ , where **L** refers to one of the capitalized spectroscopic letters. This symbol is called a *term symbol* and is placed in the upper right corner of the box. So for cobalt where the term symbol is  $^4\mathbf{F}_{9/2}$ , it means that the total spin of the electrons is  $S = 3/2$ , the total orbital angular momentum is  $L = 3$  and the total angular momentum is  $J = 9/2$ . Notice that  $J = L + S$  is the maximally allowed value.

Finally, the symbol under the atomic weight ( $[\text{Ar}]3d^74s^2$ ) is called the *electron configuration* and tells us which shells the electrons go into. For cobalt, the “[Ar]” means that the first 18 electrons go into the same shells as the electrons in Argon. The “ $4s^2$ ” means that 2 electrons go into the 4s shell, where 4 is the principle quantum number  $n$ , and “ $3d^7$ ” means that the remaining 7 electrons go into the 3d shell.

Let us now describe in some detail why the electrons fill the shells in the order that they do. Electrons are identical fermions, so by the Pauli principle no two of them can be in the same single-particle state. Let us now start filling shells sequentially. The lowest energy shell has principle quantum number  $n = 1$  and  $\ell = 0$ , so this is called **1s**. The first electron goes into this shell. The total spin for this configuration is  $S = 1/2$ , the total orbital angular momentum is  $L = 0$  and so the total overall angular momentum is  $J = 1/2$ . Since  $S = 1/2$ , there are  $2 = 2S + 1$  total spin states, so we describe this state as  $^2\mathbf{S}_{1/2}$  which you can see is the term symbol for hydrogen (**H**) which only has one electron. Hydrogen also has the electron configuration 1s below the atomic weight, telling us that the ground state has the electron in this shell. If we now add another electron, we can place one more in the 1s shell because there are two possible spins for the electrons, so we can have them in the same position state but in different spin states. Since

the electrons are in the same position state, the positional part of the wavefunction is symmetric, meaning that the spin part must be antisymmetric. Hence the total spin of the two electrons is  $S = 0$ , the total orbital angular momentum is  $L = 0$  and so the total angular momentum is  $J = 0$ . Hence this next symbol is  $^1\mathbf{S}_0$  which is the term symbol for helium (**He**).

The next electron has to go into an  $n = 2$  state since the  $n = 1$  states are now filled. The possible values for  $\ell$  are now  $\ell = 0, 1$  and for the hydrogenic atom the value of  $\ell$  does not affect the energy (fine structure corrections which depend on  $j$  will play a role, but not at this particular point.). But now we need to take into account how the charges of the electrons can affect the other electrons. The electrons in the **1s** shell are relatively close to the nucleus and their symmetric probability distribution has the effect of smearing out their negative charge over a spherical shell. In electrodynamics, the force on a charged particle outside this charged shell would be exactly the same as if all of the shell's charge were at the origin. Hence the total charge as seen by an electron outside the shell of these inner two electrons is  $(Z - 2)e$ . These inner electrons effectively screen out 2 units of charge from the nucleus. However, a charged particle inside the shell would feel no force from the shell and would only feel the force from the nucleus. Hence, in this case the nuclear charge is unscreened. The upshot of this is that an outer electron that has a greater probability of being inside the inner shell will have lower energy because it is more likely to feel an unscreened nucleus. It turns out that the lower the value of  $\ell$ , the greater the probability to be inside the shell (there will be a tutorial problem related to this.) Therefore, the next two electrons will go into the **2s** shell. The two electrons in the **1s** shell contribute nothing to the angular momenta, which is a general feature of the electrons in a filled shell, and so the next elements lithium (**Li**) and beryllium (**Be**) will have the same term symbols as **H** and **He** and with very similar electron configurations.

The next shell to start filling is the **2p**. The first four electrons contribute nothing to the angular momenta (they are in filled shells), hence for the fifth electron we have  $S = 1/2$ ,  $L = 1$ . The total angular momentum can be  $1/2$  or  $3/2$ , but as we have previously seen,  $J = 1/2$  is energetically favored by the spin-orbit interaction appearing in the fine structure. Hence, the term symbol for boron (**B**) is  $^2\mathbf{P}_{1/2}$ .

For the sixth electron we face some choices. We now have two electrons in the **2p** shell and they must combine to make an antisymmetric state. If the total spin is  $S = 1$  then the spin part of the state is symmetric and so the spatial part of the state must be antisymmetric. In this case  $L = 1$ . If the total spin is  $S = 0$  then the spin part is antisymmetric and so the spatial part must be symmetric, giving either  $L = 2$  or  $L = 0$  (see the tutorial exercise). We now invoke

**Hund's first rule:** *All else being equal, the electrons in the outer shell maximize their total spin  $S$  to lower their energy.*

Surprisingly, the physics behind this rule had been somewhat misunderstood until the 1970's when using computers it was possible to find good numerical approximations to the electron wave-functions. It is now understood that by having the largest value for  $S$ , the resulting spatial wave-function for the electrons in the outer shell favors a larger angular separation between the electrons. Thus, the nuclear charge as seen by one electron is less likely to be screened by the other electrons and so the energy is lowered. In any case, for carbon this gives  $S = 1$  and so the only possibility for the orbital angular momentum is  $L = 1$ . The total angular momentum is decided by the spin-orbit coupling which favors the orbital and spin angular momentum being anti-aligned and so  $J = |L - S| = 0$ . The term symbol for carbon is then  ${}^3\mathbf{P}_0$ .

For nitrogen (**N**), Hund's first rule gives  $S = 3/2$ . The spin part of the wave-function is completely symmetric for the three outer electrons, so the spatial part must be antisymmetric. The only possibility for the orbital angular momentum with this property is  $L = 0$  (see tutorial exercise), hence the nitrogen term symbol is  ${}^4\mathbf{S}_{3/2}$ .

When we reach oxygen (**O**) we have 4 outer electrons but only three **p** orbitals to put them in. Hence, we can not make a wave-function that is completely symmetric in the spin. The best we can do is symmetrize those spins that are in the singly filled orbitals and antisymmetrize the two spins which are in the double filled orbital. Hence the total spin is  $S = 1$ . The total orbital angular momentum is  $L = 1$ , with the three different values for  $m_L$  determined by which orbital is doubly filled. Again spin-orbit coupling determines the value of  $J$ . But if the shell is more than half-filled, then a maximum value  $J = L + S$  is favored. This is summed up in

**Hund's third rule:** *For a shell that is half-filled or less, the minimum value of  $J$ ,  $J = |L - S|$  minimizes the energy. When the shell is more than half-filled, the maximum value of  $J$ ,  $J = L + S$  minimizes the energy.*

Applying this rule to oxygen then gives  $J = 2$  and so the term symbol is  ${}^3\mathbf{P}_2$ . Since there is a third rule there must be a second rule, but we have not needed it yet so I am deferring it to later.

One more electron gives us fluorine (**F**) which has a maximum value of  $S = 1/2$ . The value of  $L$  can only be  $L = 1$ , Hund's third rule gives  $J = 3/2$  and so its term symbol is  ${}^2\mathbf{L}_{3/2}$ . Putting in one more electron gives us the last element in the second row, neon (**N**). Here all the **2p** orbitals are doubly filled and so the total spin is  $S = 0$ . It is also clear that  $L = 0$  and so  $J = 0$

and the term symbol is  $^1\mathbf{S}_0$ . Notice that this is always the term symbol for an element that completes a shell.

We have not yet given a physical explanation for the second part of Hund's third rule, so let us do that now. Notice that in filling the  $2\mathbf{p}$  shell from  $\mathbf{Be}$  to  $\mathbf{Ne}$  that the  $S$  and  $L$  parts of the term symbols follow the same pattern going forward or backward. Only the  $J$  symbol does not obey this symmetry. Instead of going from  $\mathbf{Be}$  to  $\mathbf{Ne}$  by adding electrons, we could have gone the opposite direction by taking away electrons. Each absence of an electron is called a *hole*. The holes themselves, while not actually particles, have properties similar to particles and are called *quasiparticles*. Let us add a hole to  $\mathbf{Ne}$ , giving us  $\mathbf{F}$ . The hole is itself a spin  $1/2$  quasiparticle, so  $\mathbf{F}$  has  $S = 1/2$  and the resulting value of  $L$  must be  $L = 1$  since we took one electron away with  $\ell = 1$  from a state that had  $L = 0$ . But again, we can interpret this as the hole having orbital angular momentum  $\ell = 1$ . Now the hole also has a spin-orbit coupling. But the hole is positively charged, and so the spin orbit coupling favors a maximal value for  $J$  since the magnetic moment term in the spin-orbit coupling changes sign. We can keep applying this principle as we add holes until the number of holes is half-filled, which of course is the same as being half-filled with electrons.

We now move to principle quantum number  $n = 3$ . The  $3\mathbf{s}$  and the  $3\mathbf{p}$  shells are filled exactly as for  $2\mathbf{s}$  and  $2\mathbf{p}$ . Notice that the term symbols in the third row are exactly the same as the term symbols in the second row. In fact the outer electrons are largely responsible for the chemical properties of the atoms, and so two elements in the same column have similar chemical properties.

After  $3\mathbf{p}$  it would seem that  $3\mathbf{d}$  with orbital angular momentum  $\ell = 2$  would be next in line. But now, the screening effect is so large, that it is actually energetically more favorable to fill the  $4\mathbf{s}$  shell first. After potassium ( $\mathbf{K}$ ) and Calcium ( $\mathbf{Ca}$ ) we then have scandium ( $\mathbf{Sc}$ ) which has one electron in the  $3\mathbf{d}$  shell. This has  $S = 1/2$  and  $L = 2$ . Hund's third rule then gives  $J = 3/2$  and so its term symbol is  $^2\mathbf{D}_{3/2}$ . Adding one more electron to the  $3\mathbf{d}$  shell results in Titanium  $\mathbf{Ti}$ . Hund's first rule gives  $S = 1$ . Since  $S = 1$ , these two outer electrons are in a symmetric spin state, so the spatial part of the wave-function must be antisymmetric. It turns out that there are two values of  $L$  that are antisymmetric,  $L = 1$  and  $L = 3$ . To decide which one to use, we now turn to

**Hund's second rule:** *All else being equal, after maximizing their total spin the electrons in the outer shell maximize their total orbital angular momentum to lower their energy.*

The rules should be applied in order. Hence, for titanium we find  $S = 1$  (first rule)  $L = 3$  (second rule) and  $J = 2$  (third rule). The term symbol is then  ${}^3\mathbf{F}_2$ .

In filling out the  $3d$  shell, notice that there are elements where it is energetically more favorable to remove an electron from the  $4s$  shell and put it in the  $3d$  shell (**Cr** and **Cu**). This of course affects their term symbols. A similar phenomenon happens in the next row, but notice that Hund's rules continue to be obeyed. But like most rules, Hund's rules are made to be broken. Starting at  $Z = 58$ , cesium, we start filling the  $4f$  shell. Notice that in this case there are two electrons in outer shells because the  $Z = 57$  (lanthanum) element started by putting an electron in the  $5d$  shell. Hence, Hund's rules would seem to favor  $S = 1$ . But instead it has  $S = 0$ . Furthermore, it does not violate the Pauli principle to have  $L = 5$ , but instead the value is  $L = 4$ . So be careful when filling  $d$  or  $f$  shells. But for filling  $p$  shells, Hund's rules work perfectly, as you can see by looking at the 6 right columns on the table, where the term symbols are identical in each column.

One final note: if you look carefully at the periodic table you will notice that many term symbols have an extra "o" on them, *e.g.* the term symbol for boron is actually  ${}^2\mathbf{P}_{1/2}^o$ . The "o" stands for "odd-parity". In three-dimensions, a parity transformation takes  $\vec{r} \rightarrow -\vec{r}$ . In spherical coordinates this corresponds to  $r \rightarrow r$ ,  $\theta \rightarrow \pi - \theta$  and  $\phi \rightarrow \phi + \pi$ . If you were to examine the spherical harmonic wave-functions you would find that  $Y_{\ell,m}(\pi - \theta, \phi + \pi) = (-1)^\ell Y_{\ell,m}(\theta, \phi)$ . Hence the single-particle states with odd values of  $\ell$  are odd under parity, while those with even values are even. If there are an odd number of electrons in odd  $\ell$  shells, then the parity of the entire system is odd. So for boron, there is one electron in a  $p$  ( $\ell = 1$ ) shell, so this has odd parity. Carbon has two electrons in a  $p$  shell, so this is even. But the "o" is superfluous since we could have figured out the parity by looking at the electron configuration. For example, from its electron configuration we learn that neptunium (Np) has five outer electrons in the  $5f$  shell ( $\ell = 3$ ), so this has odd parity.