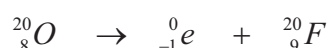


We have now seen an example with emission of alpha and gamma radiation from the decay of uranium-238 into thorium-234. In the next example the emission for beta radiation from the unstable oxygen-20 isotope will be sketched.

Example 1- F:

Emission of beta radiation

Oxygen is very well known and the stable oxygen-18 isotope is by far the most occurring oxygen isotope (8 protons and 10 neutrons in the nucleus). The oxygen-20 isotope is however not stable and it decays under the emission of beta radiation which can be sketched as follows:



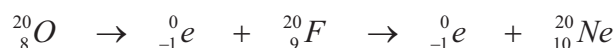
One of the neutrons in the oxygen-20 nucleus is transformed into a proton and an electron. The electron is emitted as beta radiation and because of the “extra” proton, the nucleus is now a fluor nucleus with a total of 20 nucleons. Thus the oxygen-20 isotope decays into a fluor-20 isotope. Because the electron is not a nucleon and because its mass is extremely small relative the mass of protons and neutrons, the electron is written as ${}^0_{-1}\text{e}$. The “-1” corresponds to the charge of “-1” of the electron. It is noticed that both sides of the “reaction” schema correspond, since the total number of nucleons corresponds ($20 = 0 + 20$) and the total number of charges corresponds ($8 = -1 + 9$).

It was mentioned earlier that radioactive decay often happens in *decay chains* until a stable nucleus is reached. In the following example such a decay chain will be shown.

Example 1- G:

Decay chain

As mentioned earlier radioactive decays often happen in decay chains until a stable isotope is reached. The decay of oxygen-20 can be used as an example of a decay chain:



First the unstable oxygen-20 isotope decays into the unstable fluor-20 isotope under emission of beta radiation. The unstable fluor-20 isotope then decays into the stable neon-20 isotope under emission of beta radiation. Since the last reached isotope (neon-20) is stable, the decay chain ends at this point.

A decay chain can also contain a combination of alpha, beta and gamma radiation and not just beta radiation as in the example above.

1.1.6 Wave functions and orbitals

In the section *1.1.3 Bohr's atomic model* we saw that the atomic model of Niels Bohr could not be applied to atoms with more than one electron. Thus the electrons do not move around the nucleus in circular orbits as stated by Niels Bohr. In section *1.1.4 Photons* we further saw that there is a connection between energy and mass as given by the famous Albert Einstein equation. This means that electromagnetic radiation can be considered as a stream of very small particles in motion (photons) and that particles in motion can exhibit wave characteristics. Taking that into account, electrons in motion can either be considered as particles or waves. The famous scientist Erwin Schrödinger used this to derive a mathematical model (*Schrödinger wave function*) describing the probability of finding an electron in a certain location relative to the nucleus. The Schrödinger wave function for hydrogen looks as follows:

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{8\pi^2 m}{b^2} (E - V) \Psi = 0 \quad (1-4)$$

This 2nd order differential equation looks quite nasty at first sight. However we do not have to worry about having to solve this equation because it has already been done. Solutions to this equation are the so-called *wave functions* which are denoted with the symbol Ψ . The total energy of the system is denoted E , and V is the potential energy while m is the mass of the electron. The square of the wave function (Ψ^2) gives the probability of finding the electron in a certain location relative to the nucleus. There are many solutions to such a 2nd order differential equation and each solution specifies a so-called *orbital*. An orbital is thus a certain volume or area relative to the nucleus in which the probability of finding a specific electron is given by the square of the wave function (Ψ^2). Each orbital is assigned with the following three quantum numbers:

n , primary quantum number. Can have the values 1, 2, 3, ... , ∞ . The primary quantum number says something about the size and energy level of the orbital. The larger n , the larger is the orbital and the longer away the electron is relative to the nucleus.

l , angular momentum quantum number. Can have values from 0 to $n-1$. The angular momentum quantum number tells something about the shape of the orbital.

m_l , magnetic quantum number. Can have values from $-l$ to $+l$. The magnetic quantum number tells something about the orientation of the orbital in space.

Every orbital surrounding a nucleus have a unique set of these three quantum numbers which are all integers. Hence two different orbitals can never have the same combination of these three quantum numbers. In each orbital two electrons can be hosted which leads to the introduction of a forth quantum number.

m_s , spin quantum number. Can have the value of either $-\frac{1}{2}$ or $+\frac{1}{2}$

Each of the two electrons in an orbital are thus assigned with the spin quantum number of either $-\frac{1}{2}$ or $+\frac{1}{2}$. This means that each electron in an atom is assigned with a total of four quantum numbers. The first three quantum numbers (n , l and m_l) tell which orbital the electron is placed in, while the last quantum number (the spin quantum number m_s) is just introduced in order to give each electron its unique set of quantum numbers. Since two electrons can be hosted in one orbital there is a need for the spin quantum number. The fact that

each electron has its own unique set of quantum numbers is called *Pauli's exclusion principle*. If only one electron is hosted in an orbital this electron is said to be unpaired. An element which has unpaired electrons in one or more orbitals is said to be *paramagnetic*. On the other hand an element without unpaired electrons is said to be *diamagnetic*.

Paramagnetic atom: An atom that has unpaired electrons in one or more orbitals

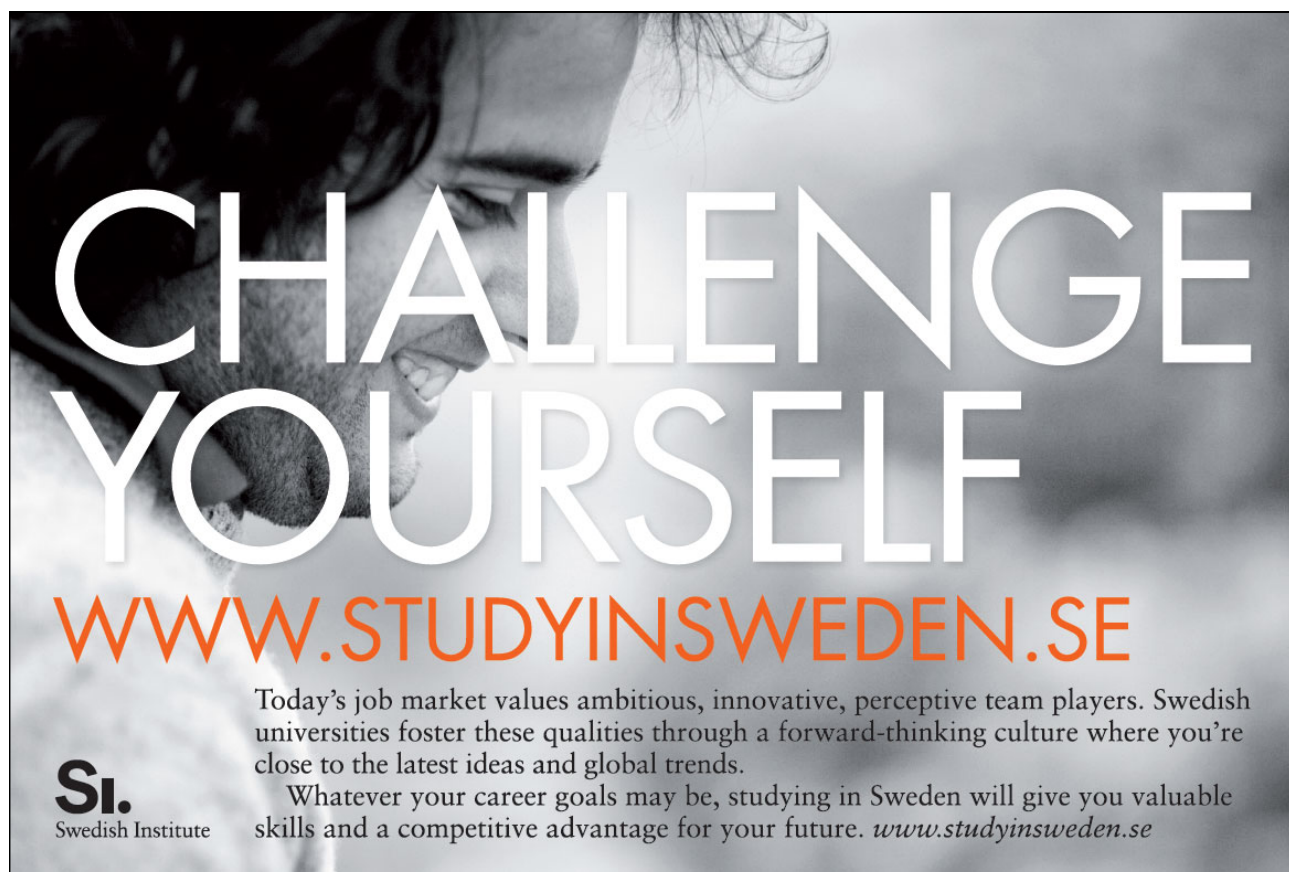
Diamagnetic atom: An atom that has *no* unpaired electrons in its orbitals.

1.1.7 Orbital configuration

As mentioned in section 1.1.6 *Wave functions and orbitals* the angular momentum quantum number l determines the shape of the orbital while the magnetic quantum number m_l determines the orientation of the orbital relative to the nucleus. Each orbital is designated with a letter dependent of the value of the angular momentum quantum number l :

$l = 0$, orbital is designated with the letter s .	$m_l = 0$	(1 orbital)
$l = 1$ orbital is designated with the letter p .	$m_l = -1, 0, +1$	(3 orbitals)
$l = 2$, orbital is designated with the letter d .	$m_l = -2, -1, 0, 1, 2$	(5 orbitals)
$l = 3$, orbital is designated with the letter f .	$m_l = -3, -2, -1, 0, 1, 2, 3$	(7 orbitals)

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Although the angular momentum quantum number l can attain larger values than “3” (there should thus be more than the four orbital types; s , p , d and f) it is only in those four mentioned types of orbital electrons are hosted. In Figure 1- 4 sketches of the s -, p - and d -orbitals are shown.

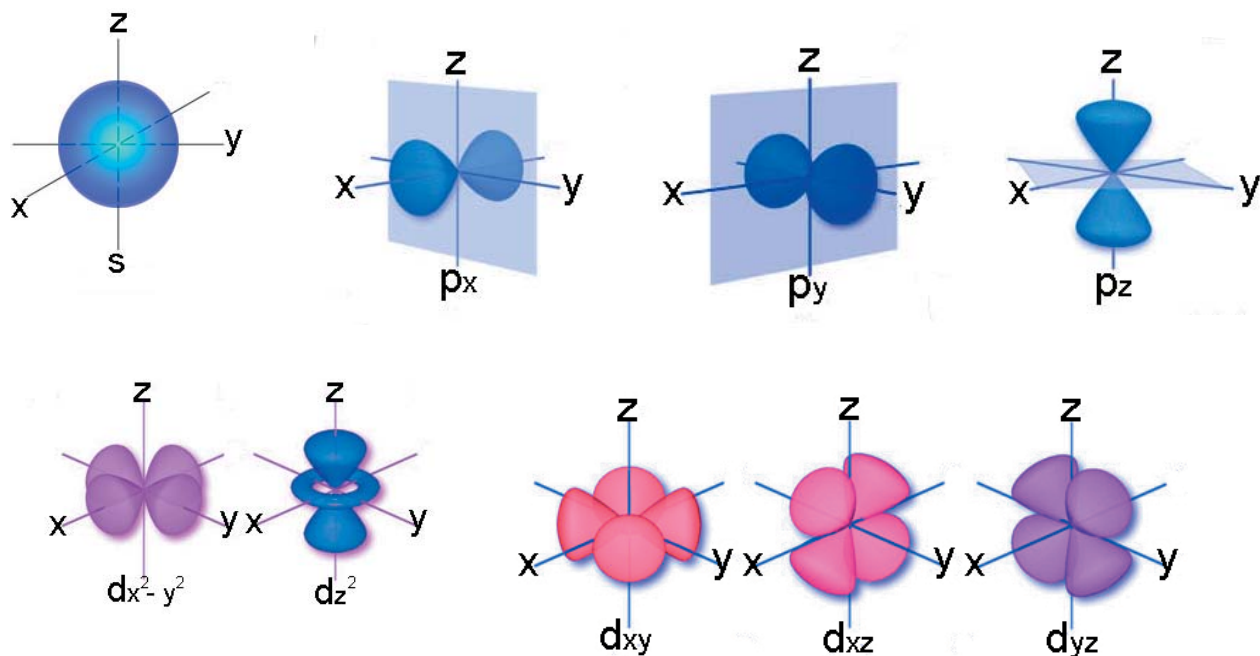


Figure 1- 4: Geometry of the orbitals

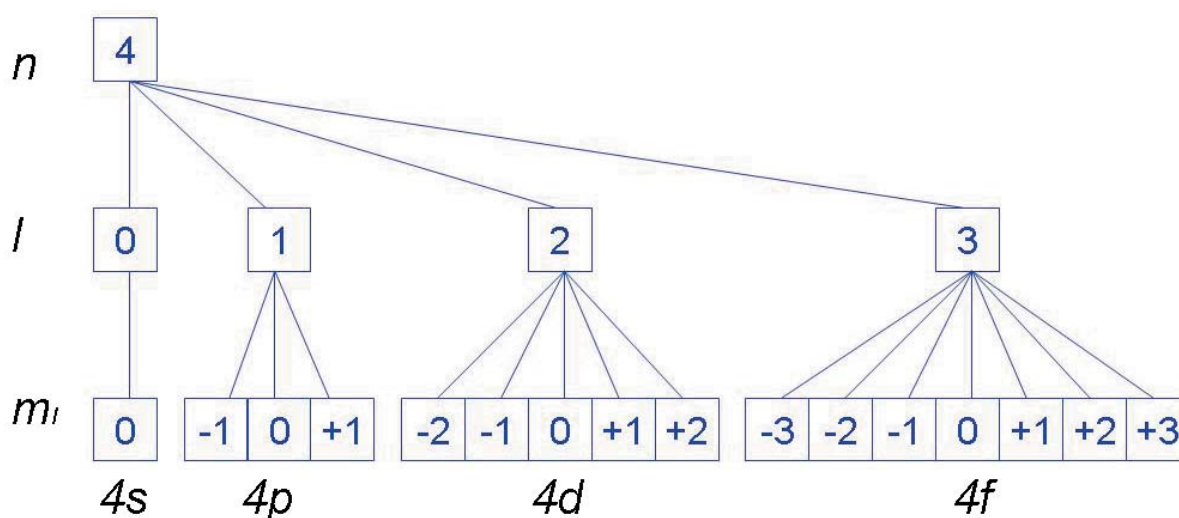
Sketch of the one s -orbital, the three p -orbitals and the five d -orbitals. The seven f -orbitals are not shown. The “names” of the different orbitals are given below each orbital.

In the following example we are going to look at the designation of letters and quantum numbers for different orbitals.

Example 1- H:*Quantum numbers and designations for different orbitals*

We are going to list the different possible quantum numbers when the primary quantum number n has the value of 4. We are also going to assign the orbitals with letter symbols.

When $n = 4$, the angular momentum quantum number l can assume the values of 0, 1, 2 or 3. For each value of l the magnetic quantum number m_l can attain the values from $-l$ to $+l$. This is sketched in Figure 1- 5.

**Figure 1- 5: Listing of orbitals**

The individual orbitals for the primary quantum number $n = 4$.

It is thus seen that when the primary quantum number has the value of 4 it gives a total of 16 “4-orbitals” which are the *one* 4s-orbital, the *three* 4p-orbitals, the *five* 4d-orbitals and the *seven* 4f-orbitals.

The Schrödingers wave equation has thus resulted in a theory about orbitals that host electrons. This model is, contradictory to the atomic model of Niels Bohr, also applicable for atoms with more than one electron (elements other than hydrogen). The lines in the line spectra are explained by postulating that an electron in excited state have one or more electrons that have “jumped” out in an outer atomic orbital with larger energy. When this or these electrons then “jump” back into the orbitals of lower energy, energy is emitted in the form of photons. The energy (wavelength) of these photons then corresponds to the energy difference between the two affected orbitals and hence only light with certain wavelengths can be emitted when for example element samples are burned off. This is pretty much the same principle as explained by Niels Bohr, the difference is just that the electrons are “*now*” hosted in orbitals instead of circular orbits.

It is important to emphasize that orbitals are areas/volumes in which the electrons with a certain probability can be found. Orbitals are derived from mathematical models and the concept of orbitals is developed in order to be able to explain certain characteristics of the element such as the line spectra. Thus we are talking about theoretical and mathematical description of probabilities of finding electrons in certain areas and this

description has turned out to be useful to explain certain characteristics. In chapter 2 we will see that the orbital theory is very useful in describing how different atoms join together and form chemical bonds which lead to the formation of molecules.

1.2 Construction of the periodic table

In section 1.1 *Atomic nucleus, electrons and orbitals* we saw that an atom in its ground state consists of an equal amount of electrons and protons and that the electrons are located around the nucleus in different orbitals. These orbitals have different levels of energy which determine where the individual electrons will be hosted. In this section we are going to look at how the elements are arranged the periodic table and why the periodic table has its actual configuration.

1.2.1 Aufbau principle

The elements in the periodic table are placed according to increasing atomic number. The atomic number corresponds to the number of protons in the nucleus which also corresponds to the number of electrons surrounding the nucleus in its ground state. The horizontal rows in the periodic table are called *periods*. The first period is related to the primary quantum number $n = 1$, the second period is related to the primary quantum number $n = 2$ and so on which is sketched in Figure 1- 6.

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MAIN GROUP ELEMENTS													MAIN GROUP ELEMENTS						
1st period	H																		He
2nd period	Li	Be	TRANSITION METALS										B	C	N	O	F	Ne	
3rd period	Na	Mg											Al	Si	P	S	Cl	Ar	
4th period	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
5th period	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
6th period	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
7th period	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg								
LANTHANOIDS			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
ACTINOIDS			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

Figure 1- 6: The periodic table

The dotted lines indicated the insertion of the lanthanoids and the actinoids.

Each period is finished with one of the noble gasses (He, Ne, Ar, Kr, Xe and Rn). The noble gasses are characterized by the fact that each orbital related to that specific period is filled with 2 electrons. This makes the noble gasses particularly stable and not very reactive or willing to join in chemical compounds with other elements. The periodic table is constructed according to the so-called *aufbau principle* in which the elements from number 1 to number 111 are placed periodically by “filling” and extra electron in the “next” available orbital with the lowest possible energy level. Thus one moves from the left to the right in each period during the filling of one extra electron at each position in the periodic table. The elements are thus arranged according to their so-called *electron configuration* which is a concept we are going to look more into in the following section.

1.2.2 Electron configuration

To go from one element to the next in the periodic table, one electron is “filled” in the next available orbital with the lowest possible energy level (and one more proton will be present in the nucleus). We know that each orbital is able to host two electrons. When all the orbital of one period are filled, a new period is started according to the *aufbau principle*. The last “attached” electron or electrons for that specific period are called *valence electrons* or *bond electrons*. In Figure 1- 7 you can see in which orbitals the outer electrons of a given element are hosted. For example for the 4th period you have the following order of orbitals:

$$4^{\text{th}} \text{ period orbital order : } 4s - 3d - 4p$$

It is the valence or bond electrons that are used when atoms join together and form chemical bonds and molecules. This will be described in details in chapter 2.

1st period	1s				1s
2nd period	2s				2p
3rd period	3s				3p
4th period	4s			3d	4p
5th period	5s			4d	5p
6th period	6s	4f		5d	6p
7th period	7s	5f		6d	

Figure 1- 7: Orbitals associated with the periodic table

The different outer orbitals of the different periods and groups.

The orbitals are filled with electrons according the *aufbau principle* from the left to the right in each period. The orbitals with lowest energy level are filled first. The orbitals can be ordered according to increasing energy level in the following row:

$$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 5f < 6d \quad (1- 5)$$

The orbitals with lowest energy level are filled first. The following examples sketch the electron configuration for all elements. That way the *aufbau principle* and construction of the periodic table will be clear.

Example 1- I:

Filling of electrons in the 1st period

The primary quantum number n equals 1 in the 1st period which means that only one orbital appears in this period and that this is an s-orbital (see section 1.1.7 *Orbital configuration* and Figure 1- 7 on page 30). According to Pauli's exclusion principle only two electrons can be hosted in one orbital which means that only two elements can be present in the 1st period. Element number 1 is hydrogen and its electron is placed in the 1s-orbital since this orbital has the lowest energy level according to the row presented in (1- 5) on page 30. Helium is element number 2 and its two electrons are also placed in the 1s-orbital. The electron configurations for the 1st period elements are written as follows:

$H, 1s^1$, hydrogen has 1 electron which is hosted in the 1s-orbital.

$He, 1s^2$, helium has 2 electrons which are hosted in the 1s-orbital.

Example 1- J:*Filling of electrons in the 2nd period*

The 1st period is ended when the 1s-orbital is filled. The 2nd period is then started when more electrons are added. According to the row given in (1- 5) on page 30 and to Figure 1- 7 on page 30 the filling of electrons in the 2nd period starts with the 2s-orbital. The electron configurations look as follows:

Li, $1s^2 2s^1$, lithium has 2 electrons in the 1s-orbital and 1 electron in the 2s-orbital.

Be, $1s^2 2s^2$, beryllium has 2 electrons in the 1s-orbital and 2 electron in the 2s-orbital.

Beryllium has two filled orbitals (1s- and the 2s-orbital) but this is not the end of the 2nd period since there are three 2p-orbitals to be filled before the period is ended. The filling of electrons in the three 2p-orbitals is to be started:

B, $1s^2 2s^2 2p^1$, boron has 2 electrons in the 1s-orbital, 2 electrons in the 2s-orbital and 1 electron in one of the three 2p-orbitals.

C, $1s^2 2s^2 2p^2$, carbon has 2 electrons in the 1s-orbital, 2 electron in the 2s-orbital and 2 single unpaired electrons in two of the 2p-orbitals.

According to *Hund's rule* it is most favourable in terms of energy for electrons to stay unpaired in degenerated orbitals. What does that mean?

For example the three 2p-orbitals are degenerated which means that they all have equal levels of energy. To put it another way; it does not matter in which of the three 2p-orbitals the last “attached” valence electron is placed in. *Hund's rule* implies that in terms of energy it is most favourable for the electron to be placed in an empty 2p-orbital whereby the electron remains unpaired (that way the atom will be paramagnetic according to what is stated in section 1.1.6 *Wave functions and orbitals*. When all 2p-orbitals are filled with single unpaired electrons you have the element nitrogen with the following electron configuration:

N, $1s^2 2s^2 2p^3$, according to Hund's rule each of the three 2p-orbitals are each filled with a single unpaired electron.

To get to the next element which is oxygen, an extra electron is filled in one of the 2p-orbitals. That way there are only two unpaired electrons left. The filling of electrons in the rest of the 2nd period is sketched below:

O, $1s^2 2s^2 2p^4$, 2 unpaired electrons in two of the 2p-orbitals. Paramagnetic.

F , $1s^2 2s^2 2p^5$, 1 unpaired electron in one of the $2p$ -orbitals. Paramagnetic.

Ne , $1s^2 2s^2 2p^6$, all orbitals of the period are filled and the period is ended. Diamagnetic.

The last attached electron or electrons in the period are (as mentioned earlier) called valence electrons or bond electrons. If fluor is used as an example the valence electrons are the two electrons in the $2s$ -orbital and the five electrons in the $2p$ -orbitals. The two inner electrons in the $1s$ -orbital are not valence electrons. They are called *core electrons* instead.

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