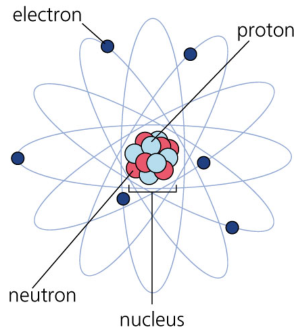
Lecture 2

The atom



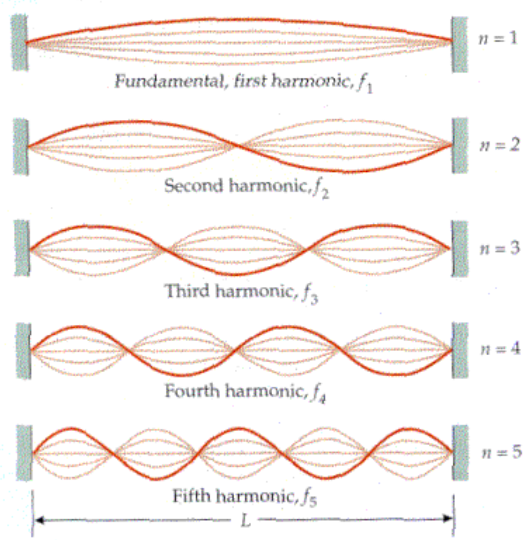
electron (negative charge)

proton (positive charge)

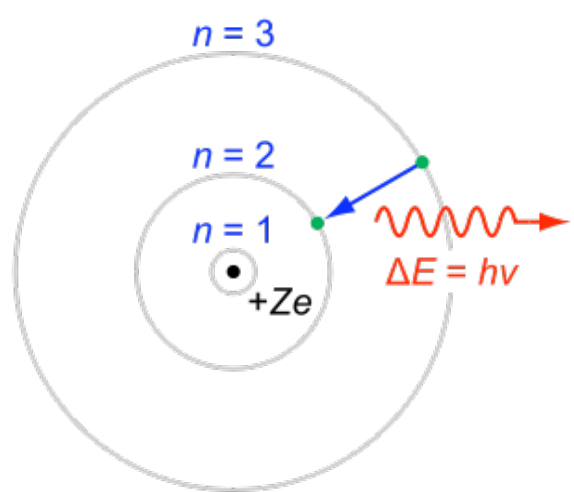
neutron (neutral)

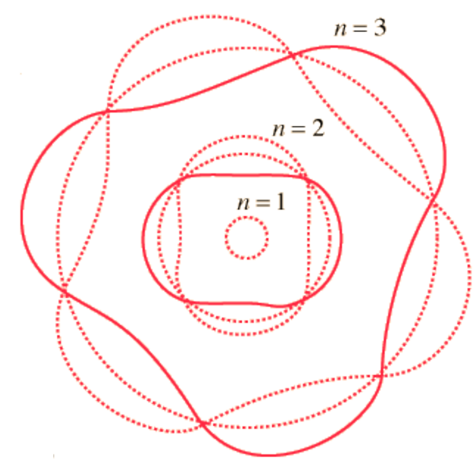
nucleus

Confined waves give quantisation



The Bohr atom



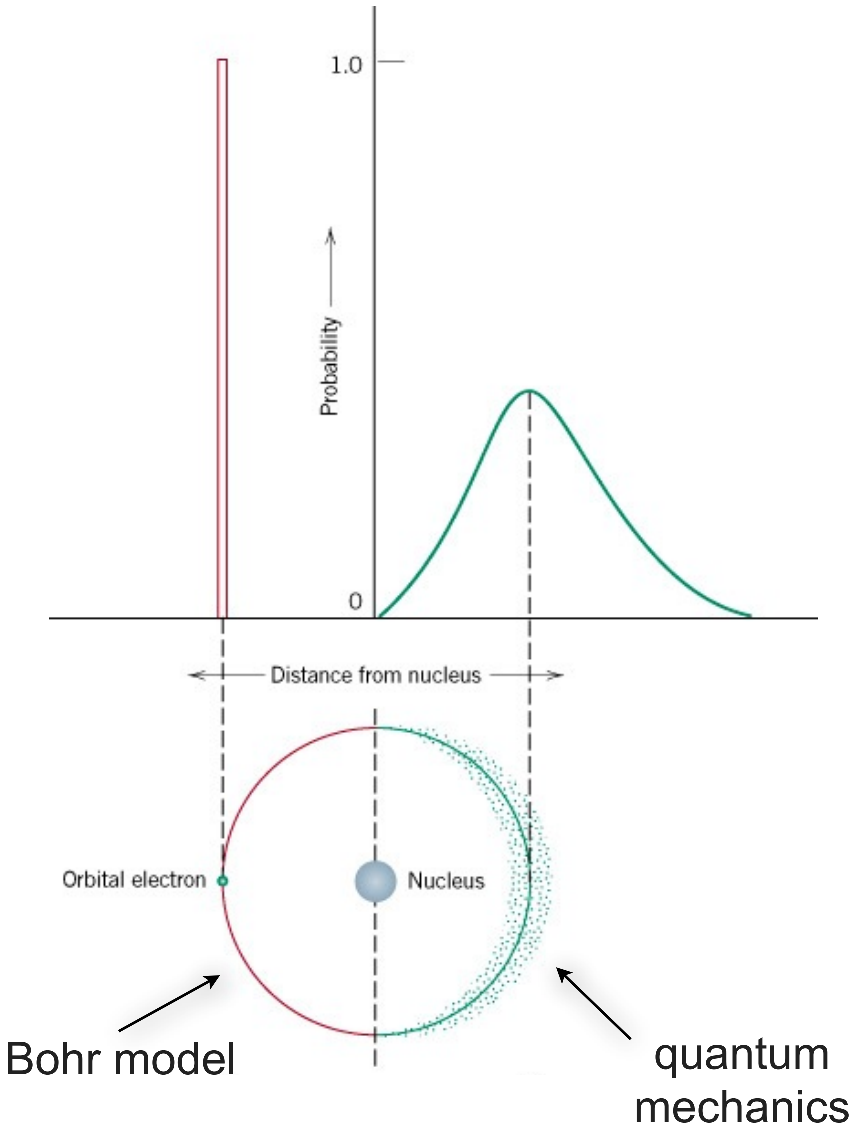


Quantum mechanics - the Schrödinger Equation

Quantum mechanics introduces a wave-function, *Ψ,* to describe the probability, *P*, that a particle occupies a particular region in space

1D: $$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2}+U(x)\psi(x)=E\Psi(x)$$

$$P(x)\propto|\ \Psi(x)\ |^2$$

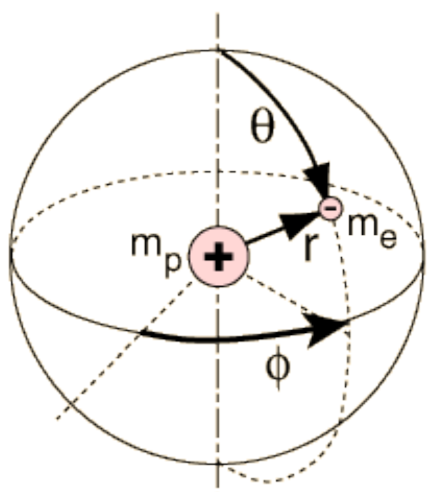


The Schrödinger Equation

3D: $$P(r,\theta,\phi) \propto |\ \Psi(r,\theta,\phi)\ |^2$$

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2\sin\theta}\left[\sin\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right)+\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right)-\frac{1}{\sin\theta}\frac{\partial^2\Psi}{\partial\phi^2}\right]+U(r)\Psi(r,\theta,\phi)$$
$$=E\Psi(r,\theta,\phi)$$

[U(r) is the potential energy of the atom, μ represents the electron mass]



$$\Psi(r,\theta,\phi) = R(r)F(\theta,\phi)$$

R(*r*): characterized by the principal quantum number, *n*

$F(\theta,\phi)$: characterized by the orbital quantum number, *l* *and* by the magnetic quantum number, m_l

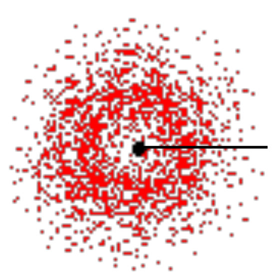
Principal Quantum Number (n) - shells

n: 1 2 3 4 5 ...

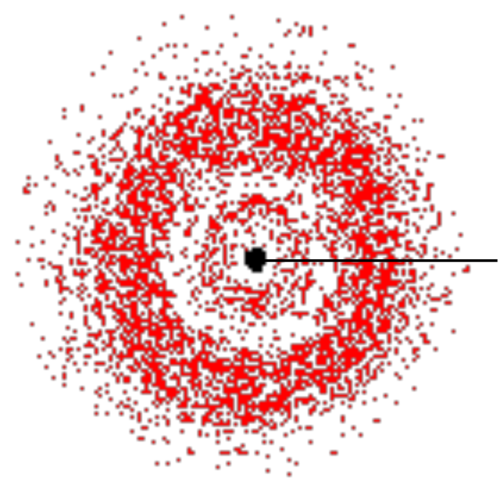
(K L M N O ...)

- Labels the atomic shell and is the same for all electrons within a shell

- The farther an electron is from the nucleus the larger n is, n represents the shell size



n=1



n=2

Subshells

The orbital quantum number: l = 0, 1, 2, 3, ... n-1 (n=the principal quantum number)

(s, p, d, f, ...)

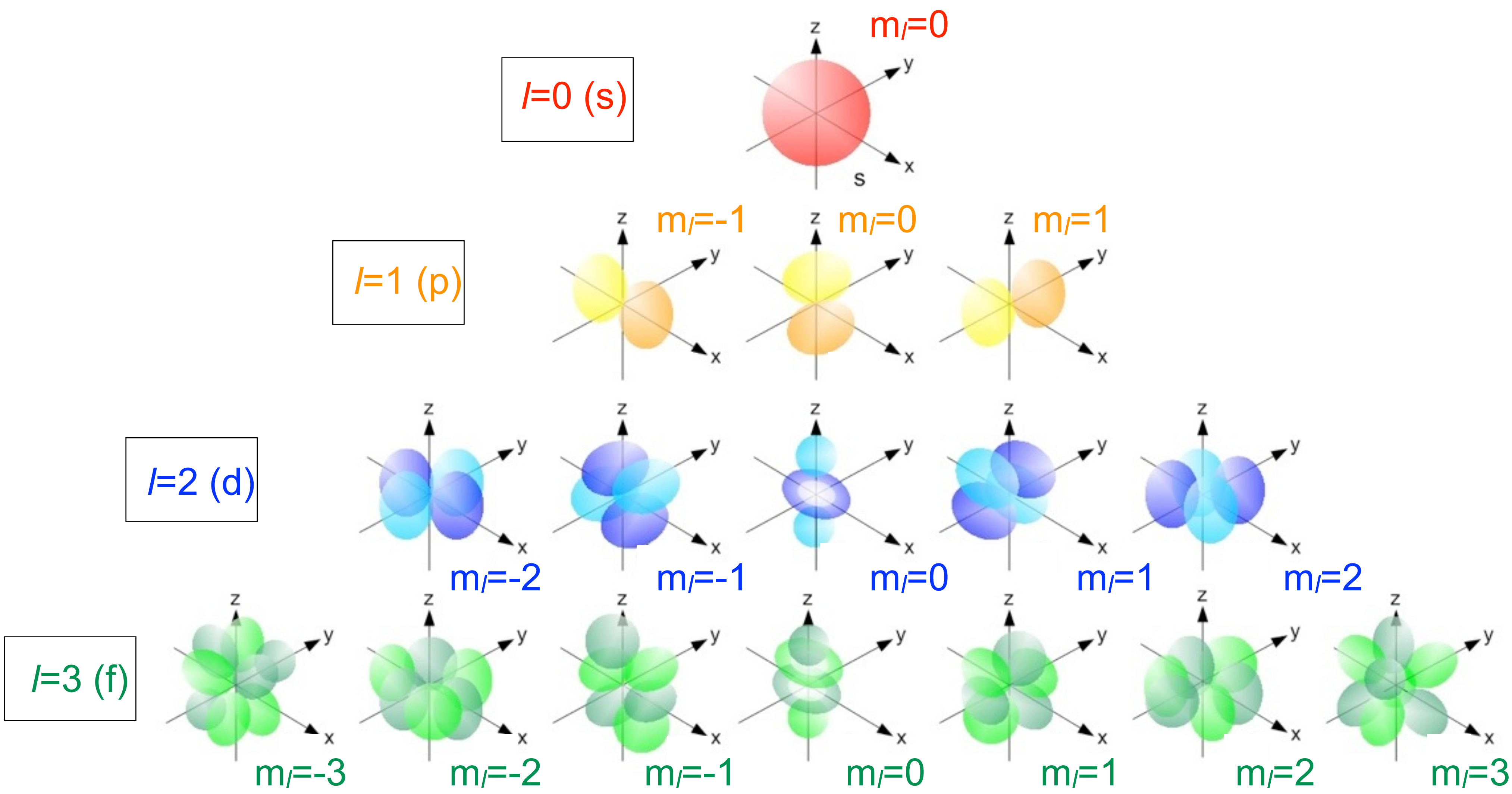
[related to the amplitude of the orbital angular momentum due to motion around the nucleus]

The magnetic quantum number: $m_l = -l, -l+1, \ldots, +l$

[related to the projection of the orbital angular momentum on a chosen axis]

[subshells with different m_l differs in energy in a magnetic field]

Electron subshell shapes

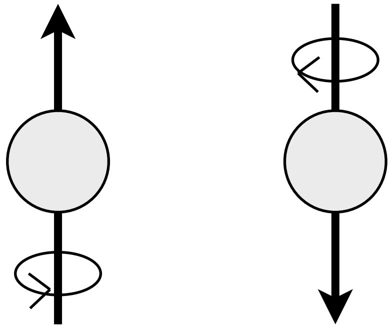


Spin

The spin quantum nr m_s = +1/2, -1/2 (spin up ↑ or spin down ↓)

[m_s relates to the electron's intrinsic angular momentum - a quantum mechanical property]

Classical spin



Electron spin is however a purely quantum mechanical property!

Quantum numbers

An electron in an atom is characterised by four quantum numbers:

1. The principal quantum number (shell): n = 1, 2, 3, ...

2. The orbital quantum nr: l = 0, 1, 2, 3, ... n-1
   (s, p, d, f, ...)

3. The magnetic quantum number: $m_l = -l, -l+1, ..., +l$ [$2l+1$ states]

4. The spin quantum nr: m_s = +1/2, -1/2

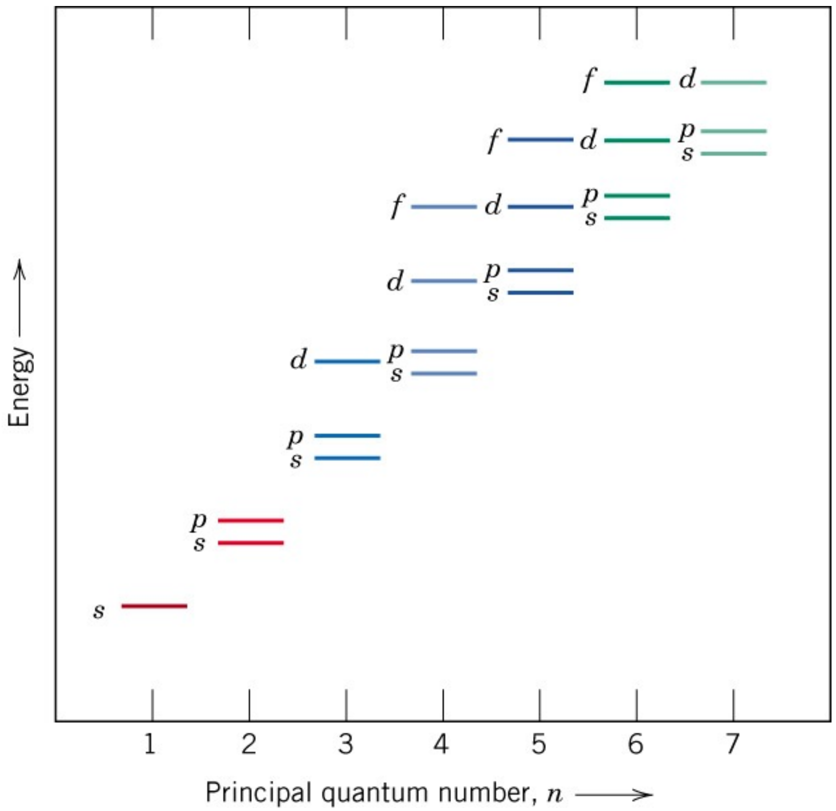
Pauli exclusion principle: only one electron is allowed in each state characterised by all four quantum numbers

Summary of electron configurations

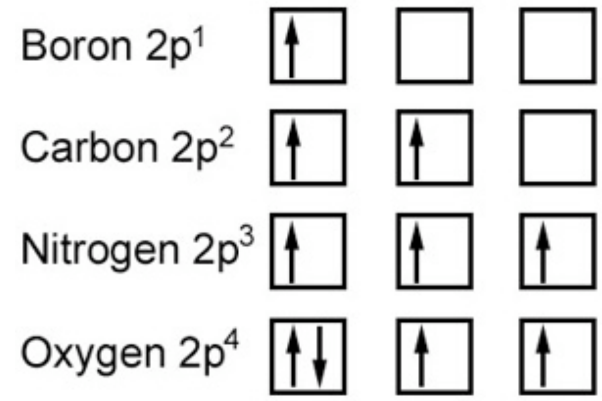
n	l	m_l	m_s	nr of electrons in subshell
1	0 [*s*]	0	±1/2	2
2	0 [*s*]	0	±1/2	2
	1 [*p*]	-1,0,1	±1/2	6
3	0 [*s*]	0	±1/2	2
	1 [*p*]	-1,0,1	±1/2	6
	2 [*d*]	-2,-1,0,1,2	±1/2	10
4	0 [*s*]	0	±1/2	2
	1 [*p*]	-1,0,1	±1/2	6
	2 [*d*]	-2,-1,0,1,2	±1/2	10
	3 [*f*]	-3,-2,-1,0,1,2,3	±1/2	14

Electronic energy levels

Energy of shells/subshells



Hund's rule

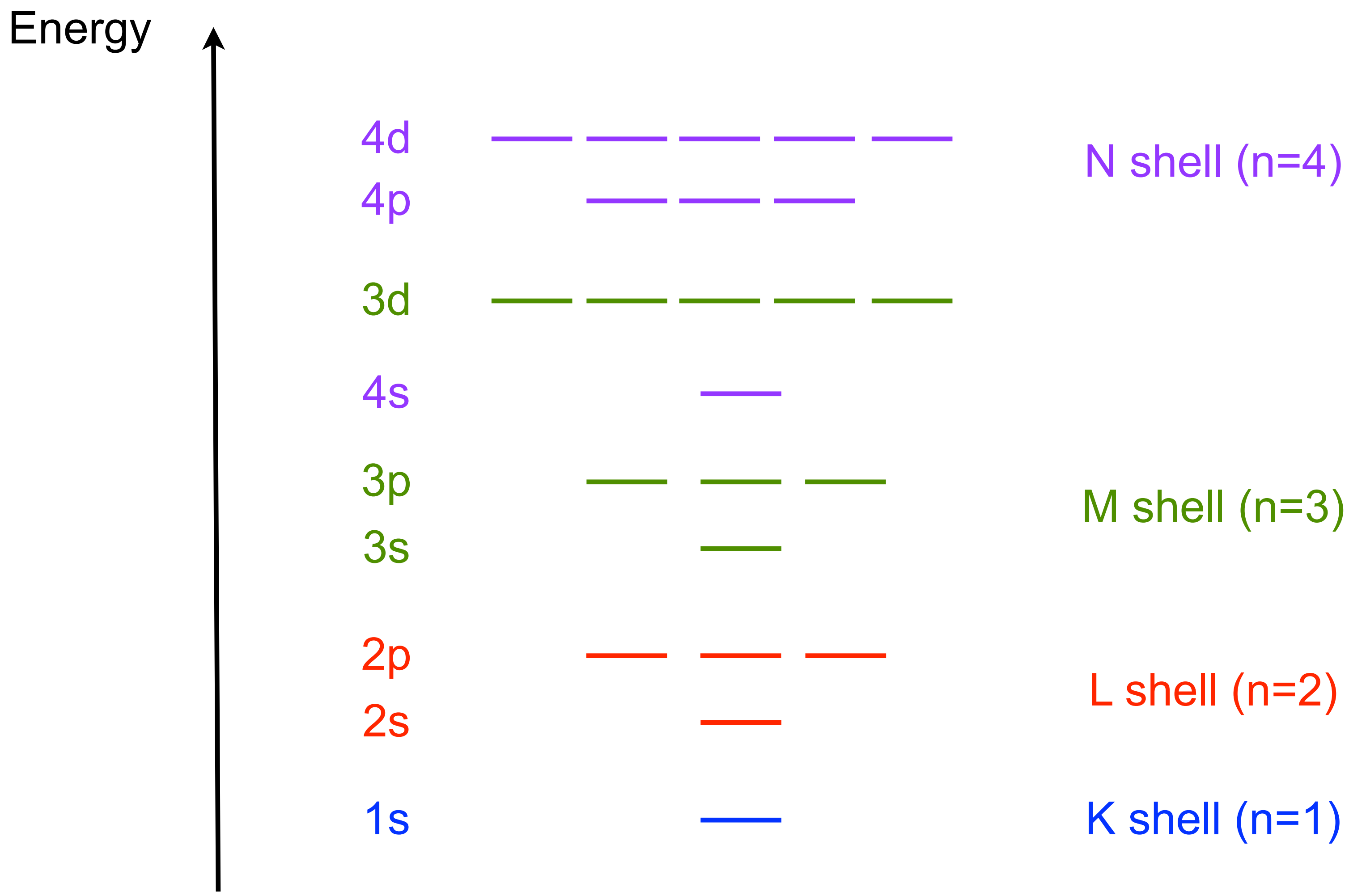


the electron configuration in an atomic ground state maximises the number of unpaired electrons

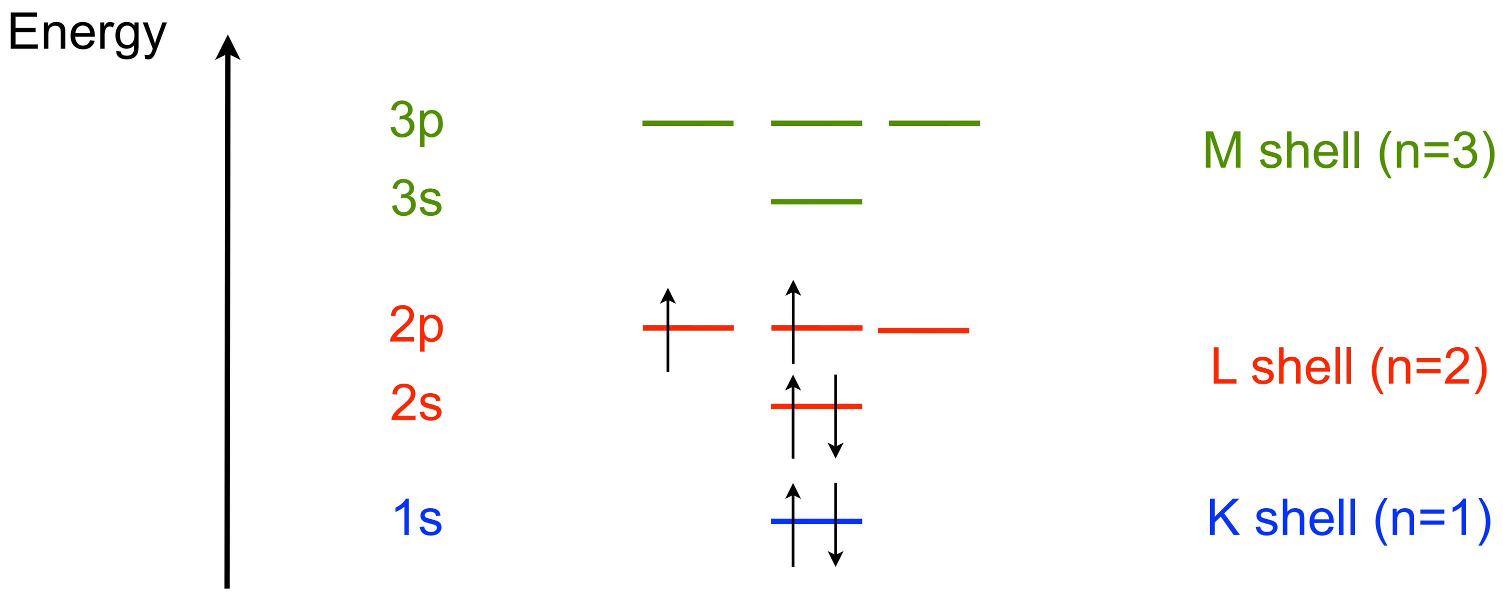
Aufbau principle

- fill orbitals starting at the lowest energies
- only two electrons (spin-up and spin-down) in each orbital
- remember Hund's rule (see above)

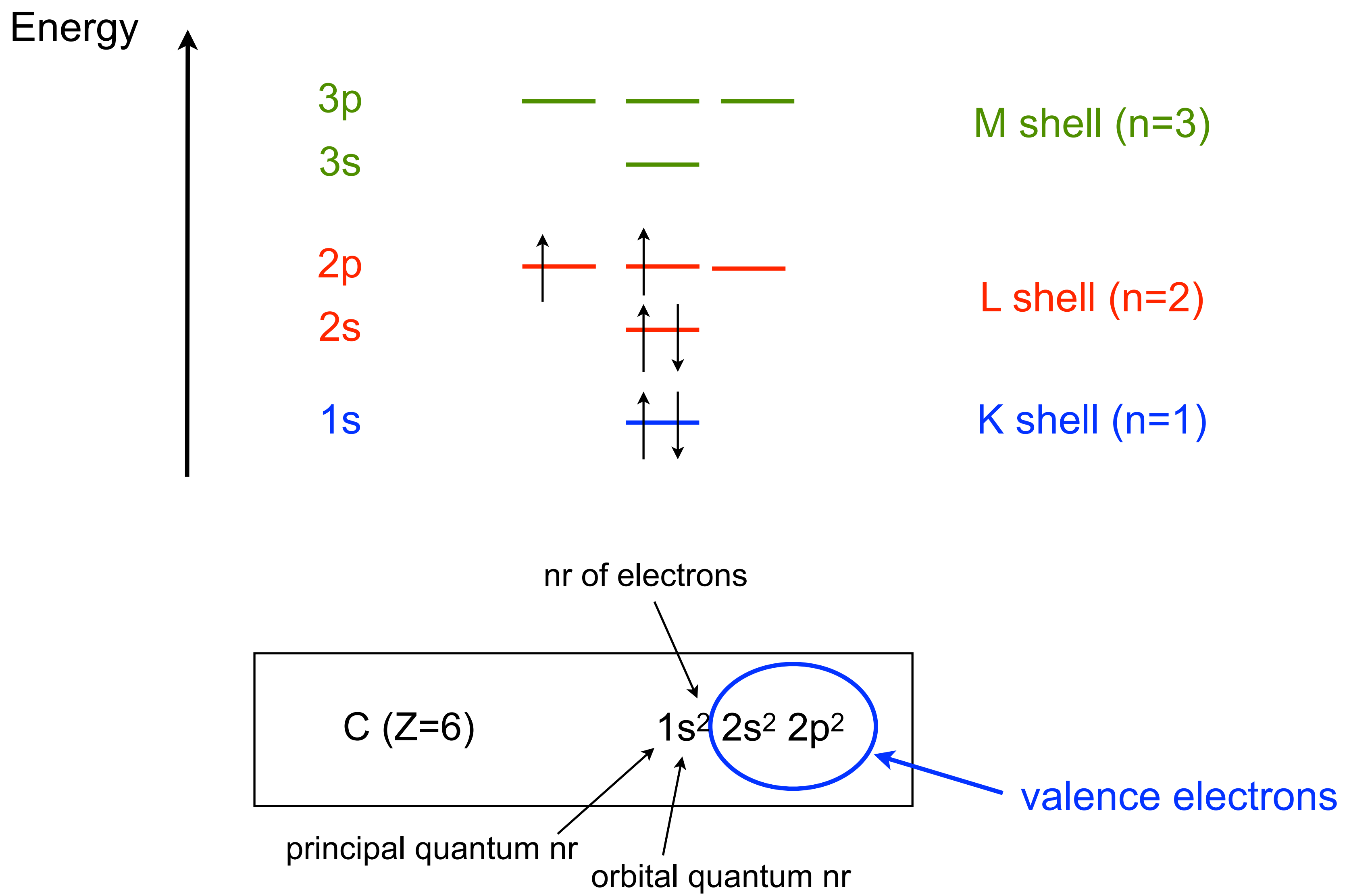
Electronic diagram



C (Z=6)

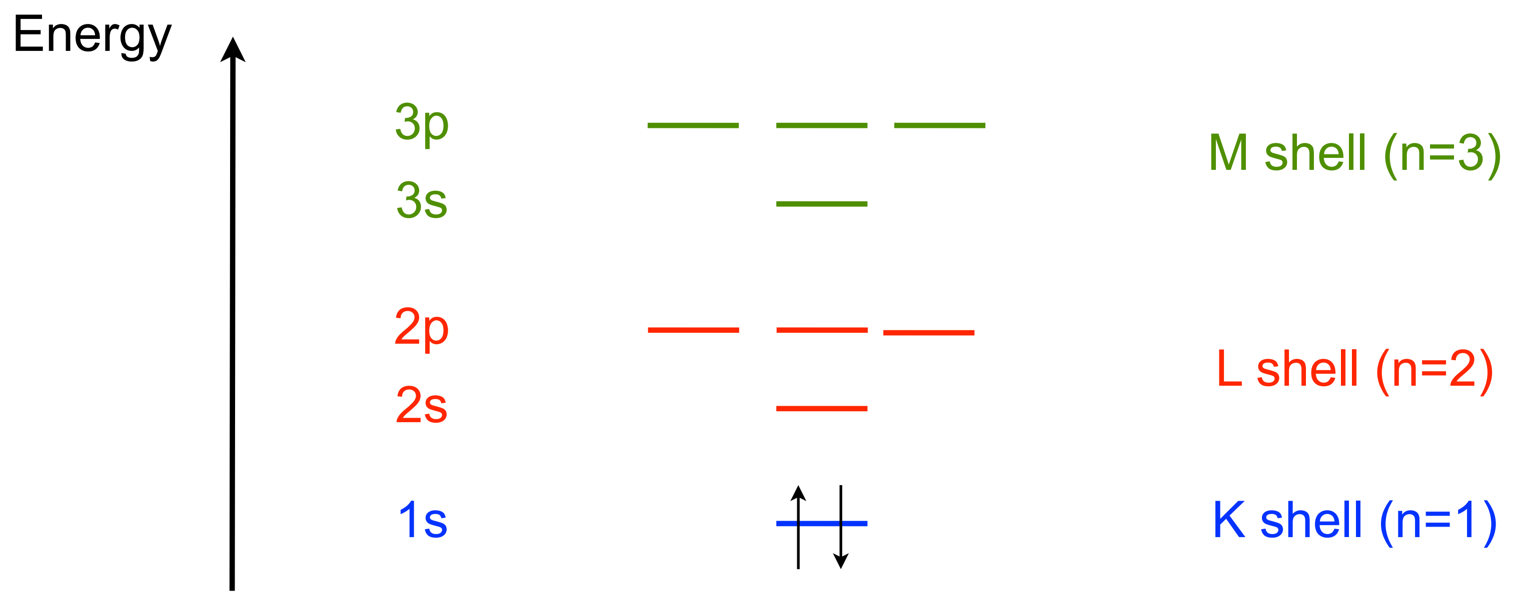


C (Z=6)



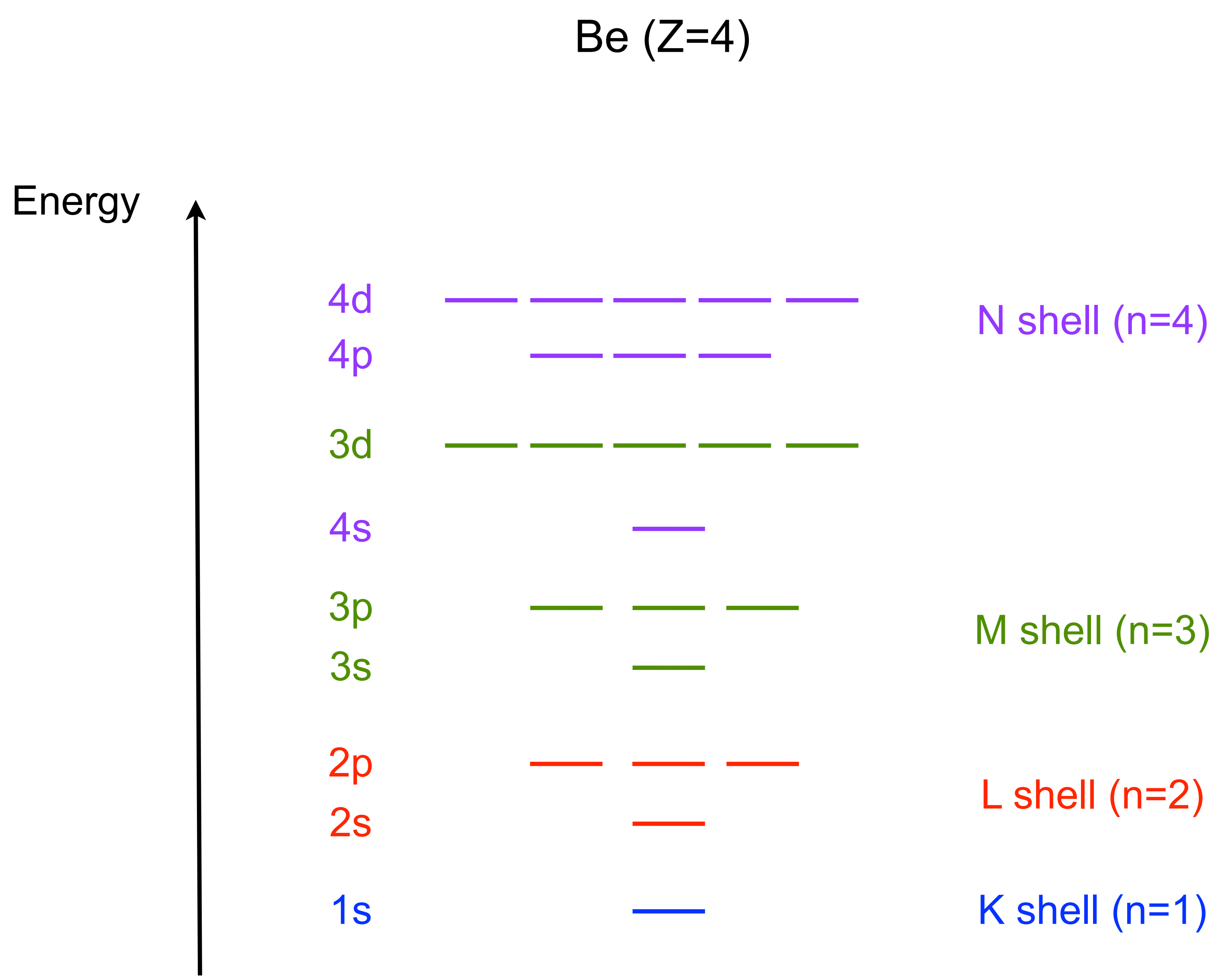
atomic number (Z): nr of protons in the nucleus= nr of electrons in neutral atoms

He (Z=2)

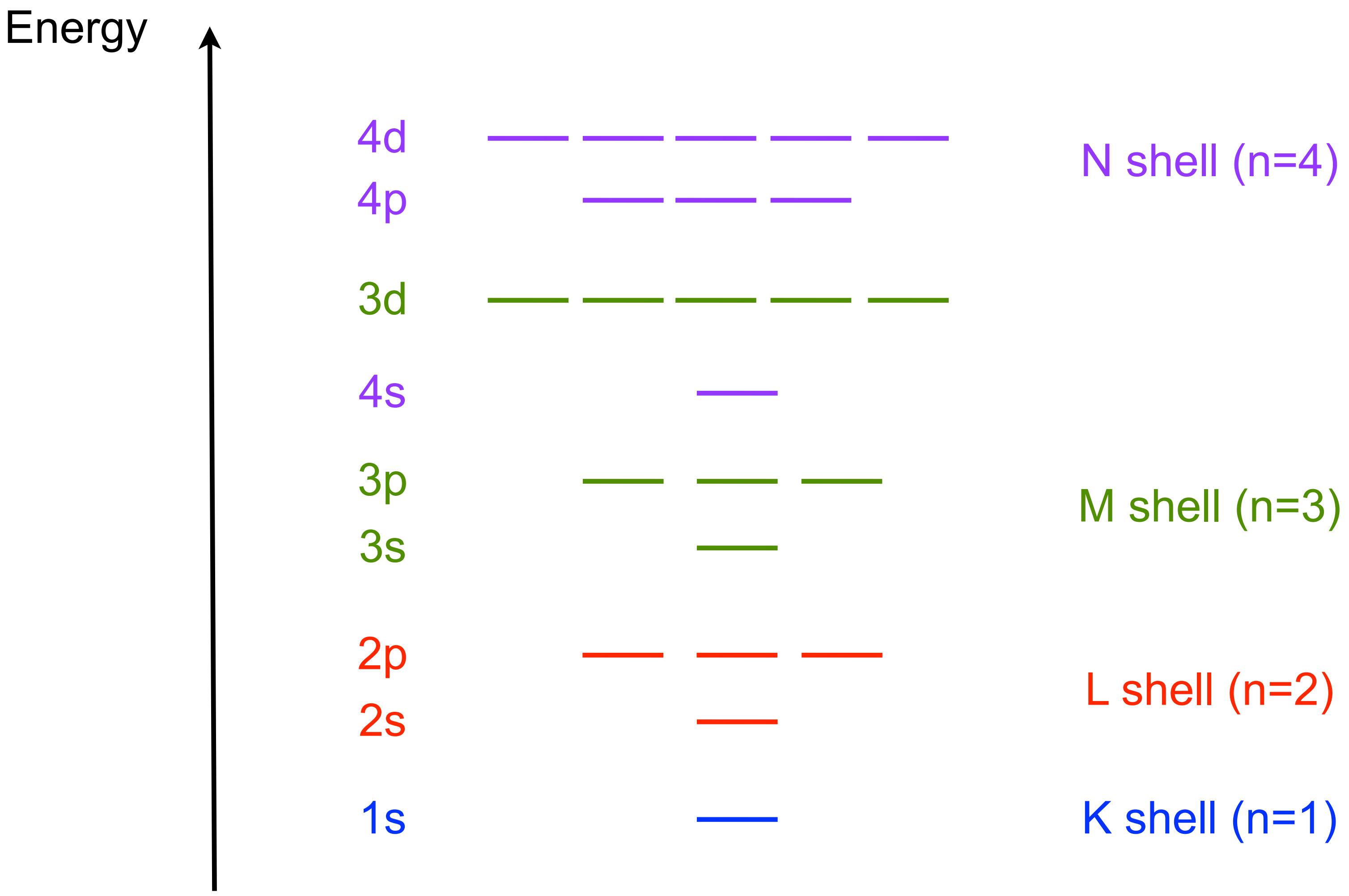


He (Z=2)	$1s^2$

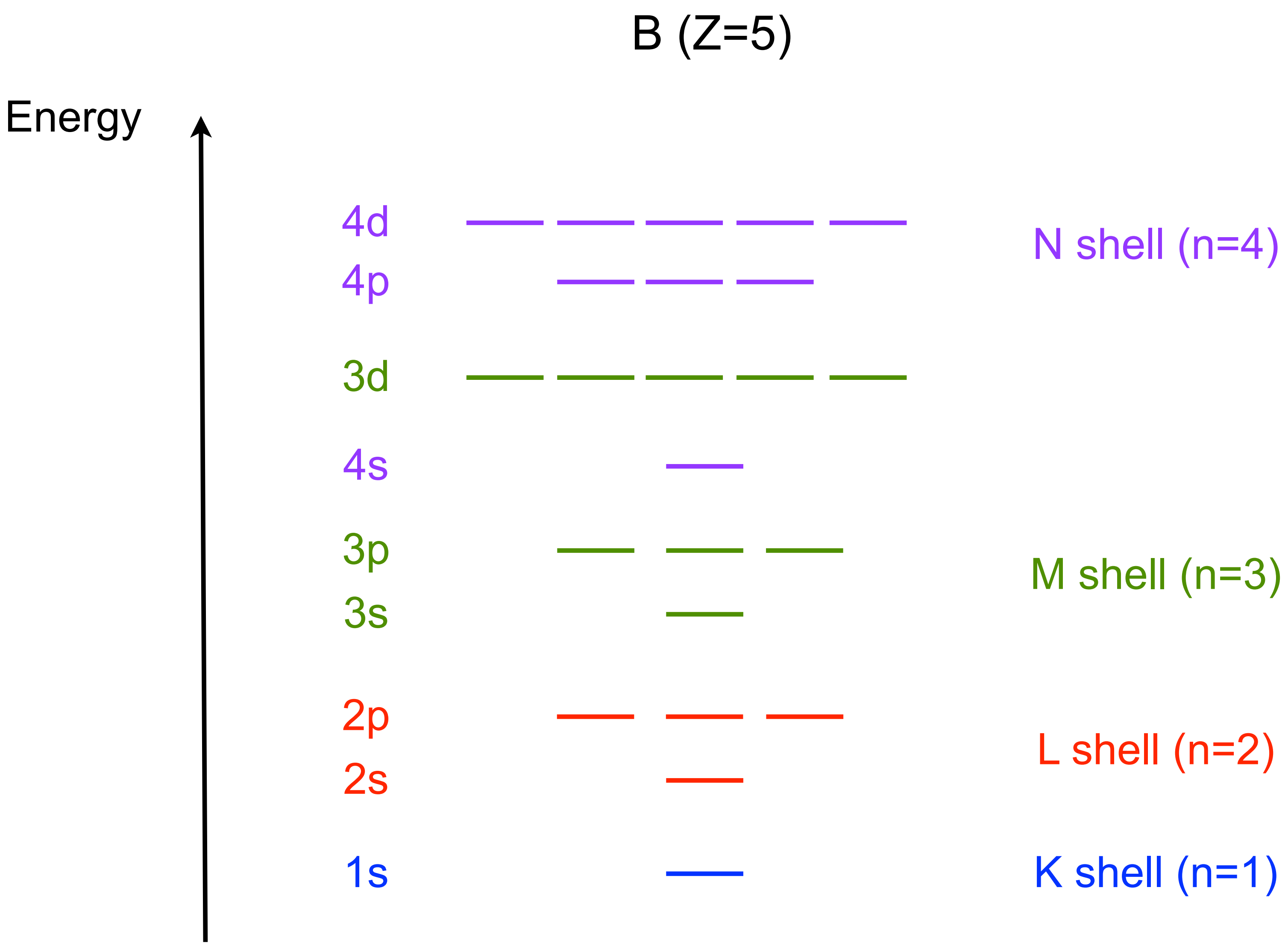
2 valence electrons!


Be (Z=4)
Energy
4d
4p
3d
4s
3p
3s
2p
2s
1s
N shell (n=4)
M shell (n=3)
L shell (n=2)
K shell (n=1)

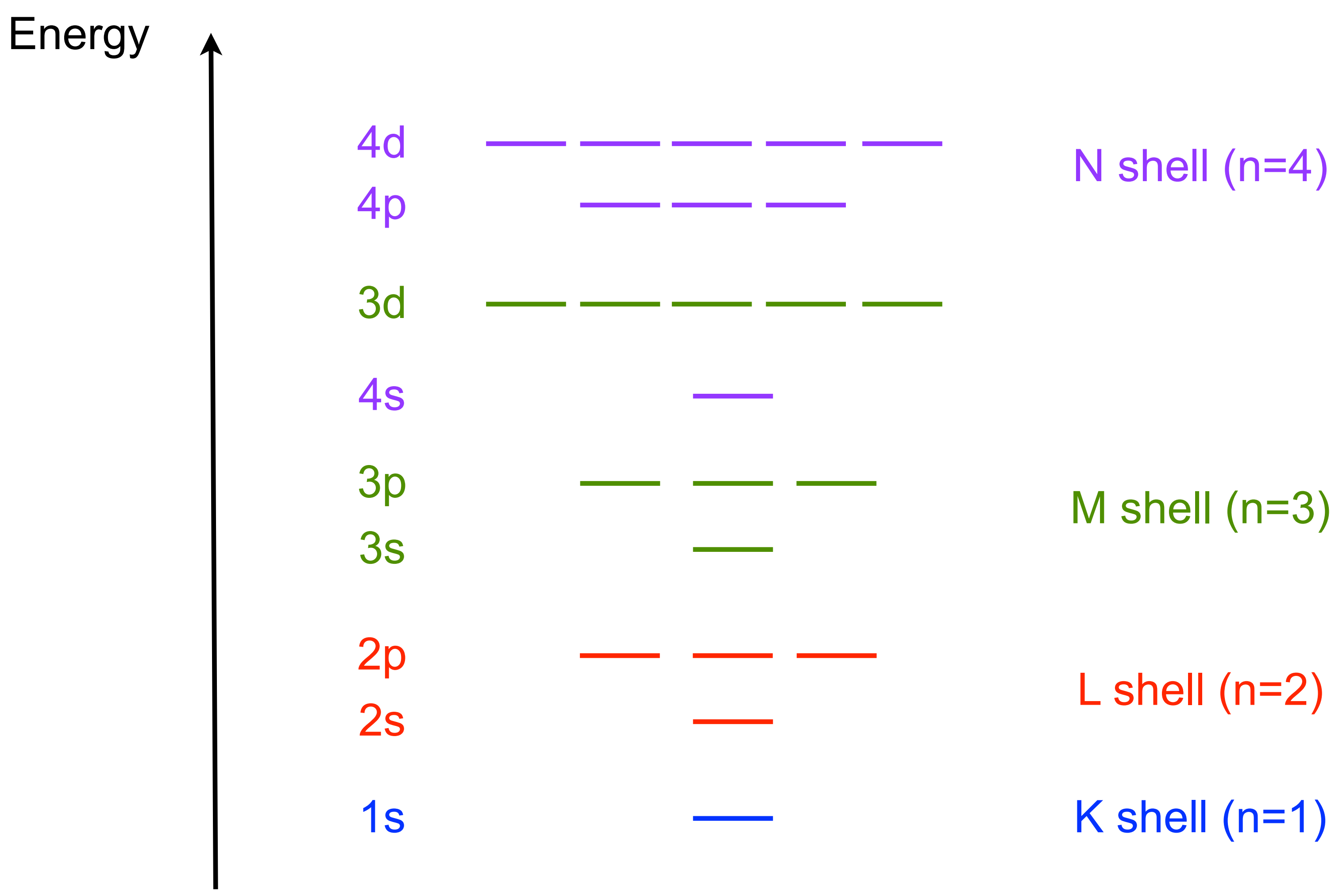
Ne (Z=10)



Energy
4d
4p
3d
4s
3p
3s
2p
2s
1s
N shell (n=4)
M shell (n=3)
L shell (n=2)
K shell (n=1)


B (Z=5)
Energy
4d
4p
3d
4s
3p
3s
2p
2s
1s
N shell (n=4)
M shell (n=3)
L shell (n=2)
K shell (n=1)

Kr (Z=36)


Energy
4d
4p
3d
4s
3p
3s
2p
2s
1s
N shell (n=4)
M shell (n=3)
L shell (n=2)
K shell (n=1)

Filled shells and valence electrons

- If a shell contains the maximum nr of allowed electrons it is termed "filled" or "closed"
- Atoms in which the outermost shell consists of a filled s and p subshell are also non-reactive and are generally also termed filled shells. A filled shell can thus mean either a truly filled shell or a shell consisting of a filled s and p subshells.
- Atoms with filled shells are chemically stable and will not easily react with other atoms
- To fill the s and p subshells of the outermost shell takes 8 electrons. The striving for this condition, to fulfil the so called octet rule, controls most of chemistry.
- The electrons in the outermost occupied shell(s) of an atom are called the valence electrons
- The valence electrons are the electrons that take part in bonding and control the chemical, thermal, electrical, optical etc properties of a material