Atomic Structure:

Quantum mechanics and electronic configuration

Quantum Mechanics

QM: Describes the arrangement of electrons in atoms in terms of:

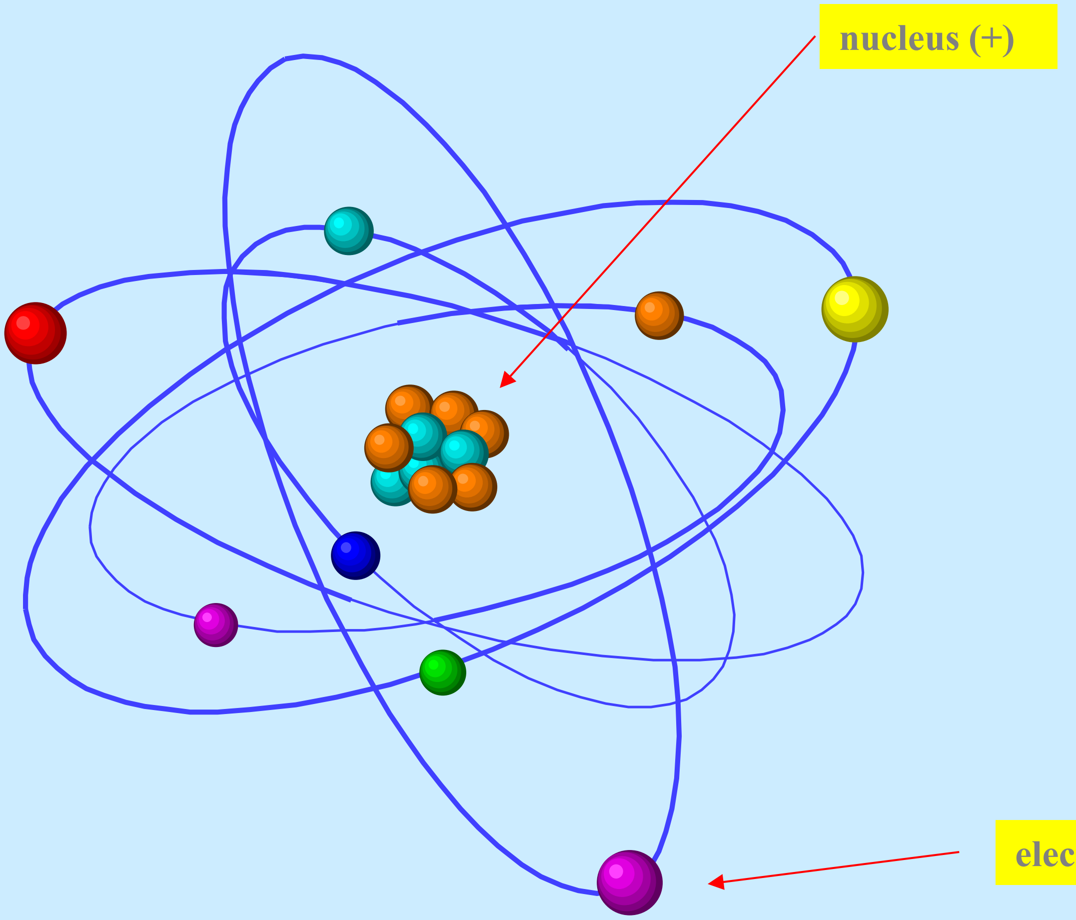
☞ **Main or principal energy levels (*n*)**

☞ **Energy subshells**

☞ **Orbitals** (space occupied within the atom)

Bohr Model of the Atom

Solar System Model has electrons moving around the nucleus.



electron (-)

Bohr Model

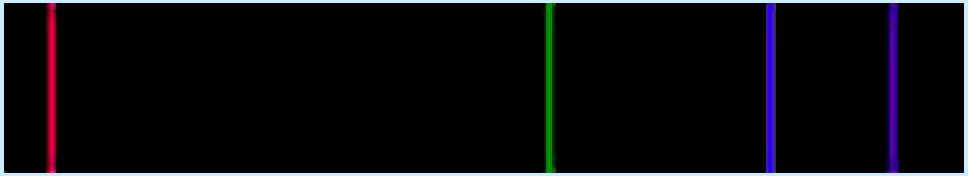
- Electrons exist only in *orbits* with specific amounts of energy called energy levels
- **Therefore…**
  - Electrons can only gain or lose certain amounts of energy
  - Only certain *photons* are produced

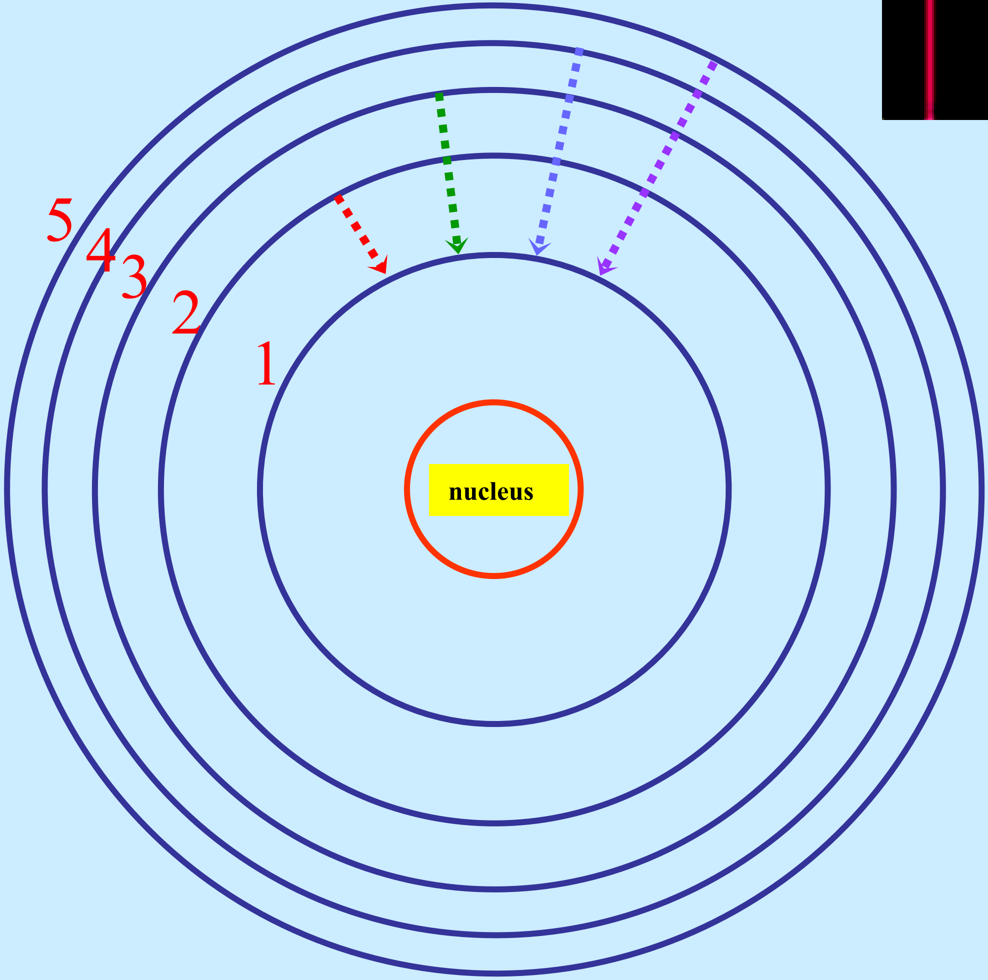
Niels Henrik David Bohr
Oct. 7, 1885 – Nov. 18, 1962
Danish Physicist

The Nobel Prize in Physics 1922 for the investigation of the structure of atoms and of the radiation emanating from them.

Bohr Model:

Proposed a model that the electron in a hydrogen atom moves around the nucleus **only in certain allowed circular orbits**.

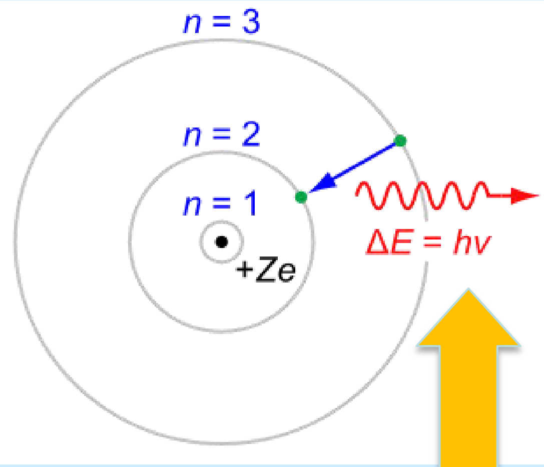




- Energy of photon depends on the **difference** in energy levels.
- Bohr's calculated energies matched the **IR**, **visible**, and **UV** lines for the **H** atom.

Quantum Mechanics

- QM better than any previous model - explain how the atom behaves.
- QM treats electrons not as **particles**, but more as **waves** (like light waves) which can gain or lose energy.

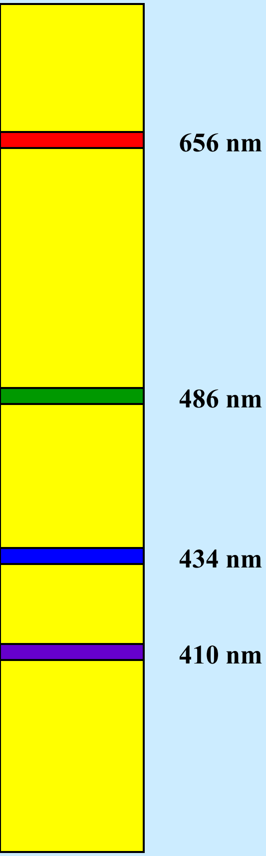


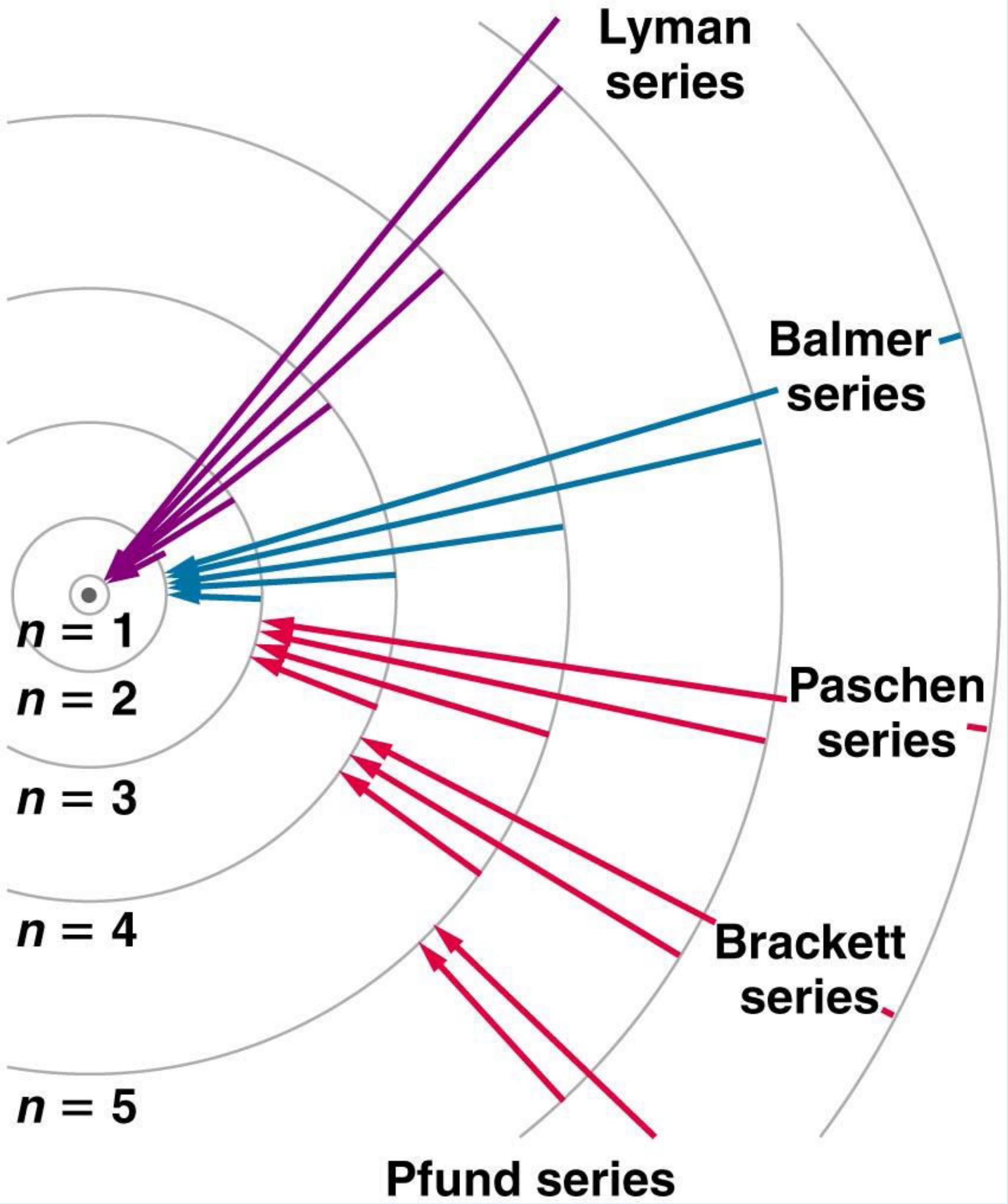
✓ But they can't gain or lose just any amount of energy. They gain or lose a "quantum" of energy.

✓ A quantum is just an amount of energy that the electron needs to gain (or lose) to move to the next energy level.

✓ QM calculates the probabilities where you are "likely" to find electrons.

HYDROGEN SPECTRAL LINES





(ultraviolet)

(visible)

(infrared)

Atomic Structure: Orbitals

Quantum mechanics:

- An electron has both **wave** and particle properties.
- Electron energies and locations can be described by a *wave equation*
  - *Wave function* solution of wave equation
  - Each wave function is an **orbital**, ψ
- A plot of ψ^2 describes where electron most likely to be.
- Electron cloud has **no specific boundary** so we show most probable area.

Quantum Numbers(QN)

- **PRINCIPAL QN:** n - energy level, the distance the orbital is from the nucleus (1, 2, 3, 4…)
- **ANGULAR MOMENTUM QN:** ℓ - shape (s = 0, p = 1, d = 2, f = 3)
- **MAGNETIC QN:** m_ℓ - spatial orientation

  0 for *s*;

  -1, 0, +1 for p;

  -2, -1, 0, +1, +2 for d, *etc.*

- **SPIN QN:** m_s - spin ($+ {}^1/_2$ or $- {}^1/_2$)

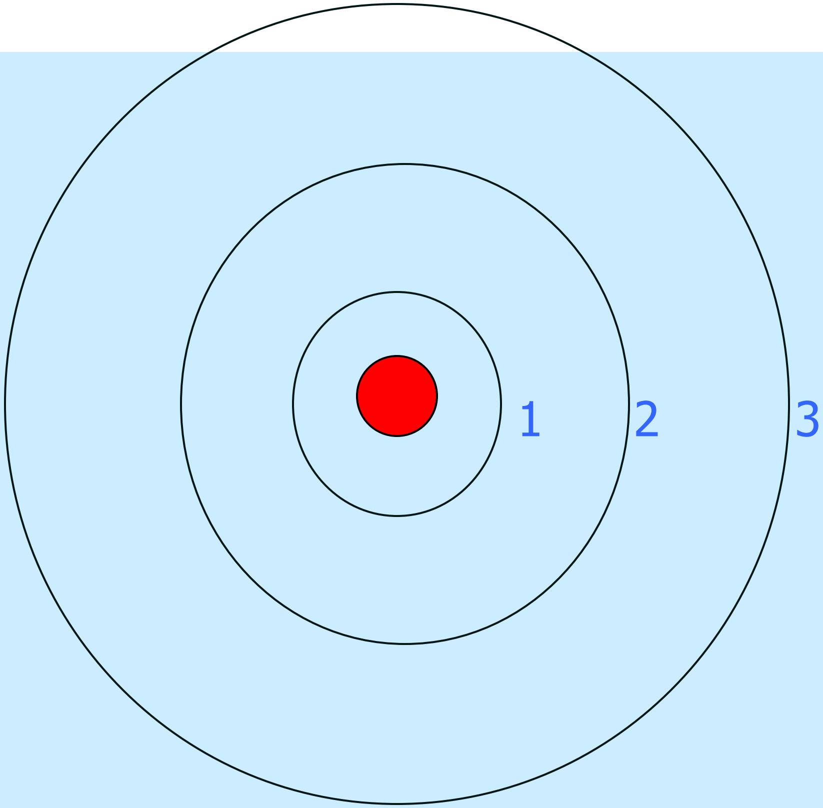
Quantum Numbers

- The principal quantum number has the symbol n.

  n = 1, 2, 3, 4, ... "shells"

  (n = K, L, M, N, ...)

  The electron's energy depends principally on n .



Angular momentum quantum number

- The angular momentum quantum number has the symbol ℓ.

  ℓ = 0, 1, 2, 3, 4, 5, ...(n-1)

  ℓ = s, p, d, f, g, h, ...(n-1)

- ℓ tells us the shape of the orbitals.
- These orbitals are the volume around the atom that the electrons occupy 90 - 95% of the time = probability density of locating an electron.

Magnetic quantum number

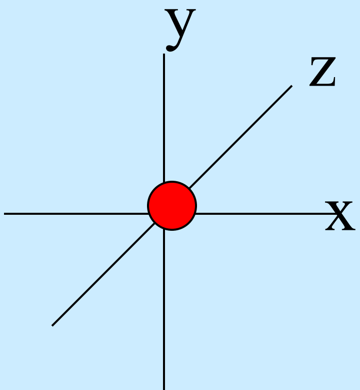
- The symbol for the magnetic quantum number is m_ℓ, **representing the spatial orientation.**

$$m_\ell = -\ell,\ (-\ell + 1),\ (-\ell + 2),\ \ldots..0,\ \ldots\ldots.,\ (\ell - 2),\ (\ell - 1),\ \ell$$

$$(\text{total} = 2\ell + 1)$$

- If $\ell = 0$ (or an s orbital), then $m_\ell = 0$ (just one orientation).

- If $\ell = 1$ (or a **p** orbital), then $m_\ell = -1, 0, +1$.



- If $\ell = 2$ (or a d orbital), then $m_\ell = -2,-1,0,+1,+2$.

- If $\ell = 3$ (or an f orbital), then $m_\ell = -3,-2,-1,0,+1,+2, +3$.

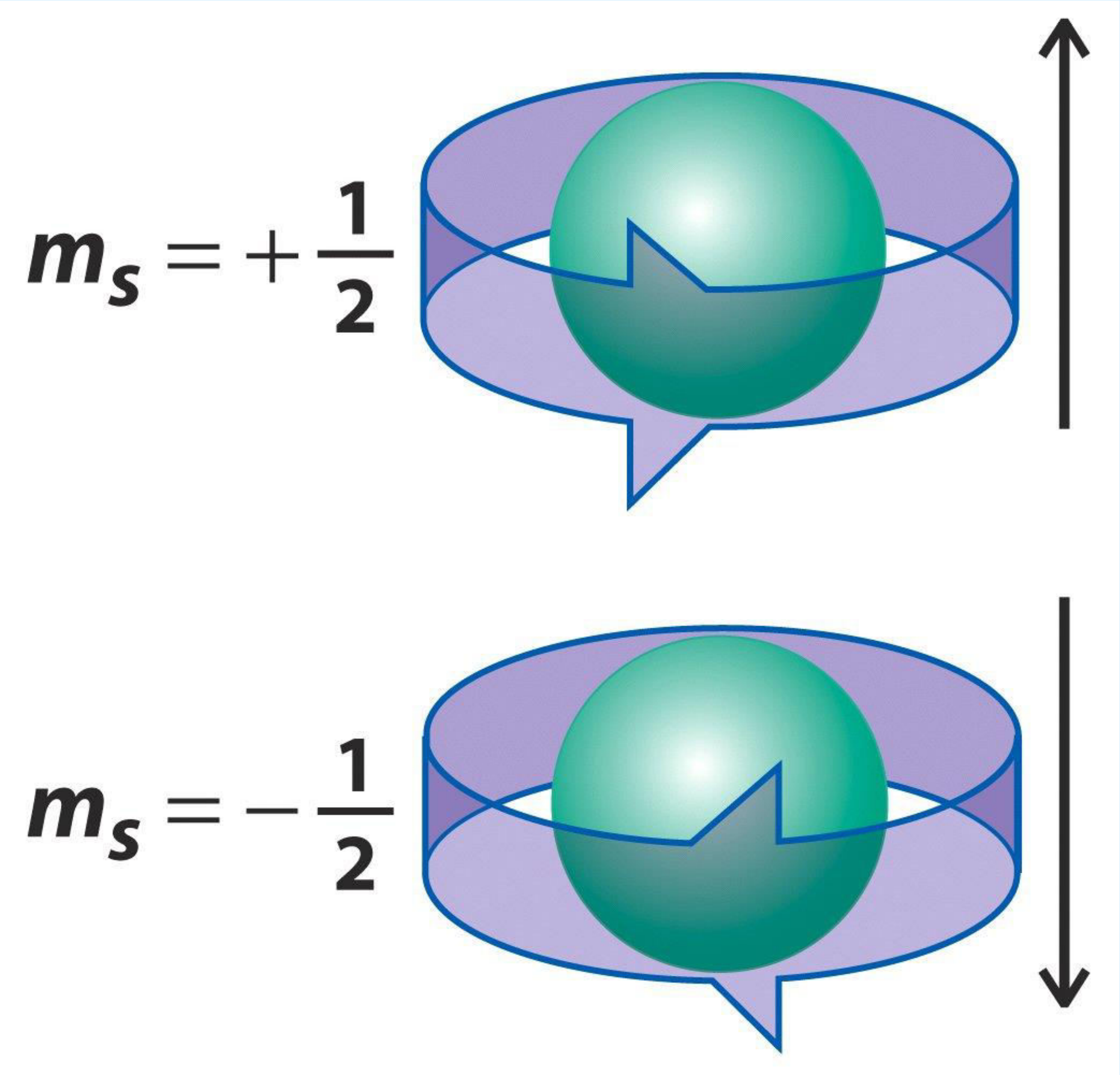
- Theoretically, this series continues on to g, h, i, *etc*

Spin quantum number

- The last quantum number is the spin quantum number which has the symbol m_s.

- The spin quantum number only has two possible values.

$m_s = +{}^1/_2$ or $-{}^1/_2$



Spin of electron

- Each energy level has 1 or more "sub-levels" which describe the specific "atomic orbitals" for that level.
  - n = 1 has 1 sub-level (the "s" orbital)
  - n = 2 has 2 sub-levels ("s" and "p")
  - n = 3 has 3 sub-levels ("s", "p" and "d")
  - n = 4 has 4 sub-levels ("s", "p", "d" and "f")

- There are 4 types of atomic orbitals:
  - s, p, d and f
  - Each of these sub-levels represent the blocks on the periodic table.

Quantum Numbers : Summary

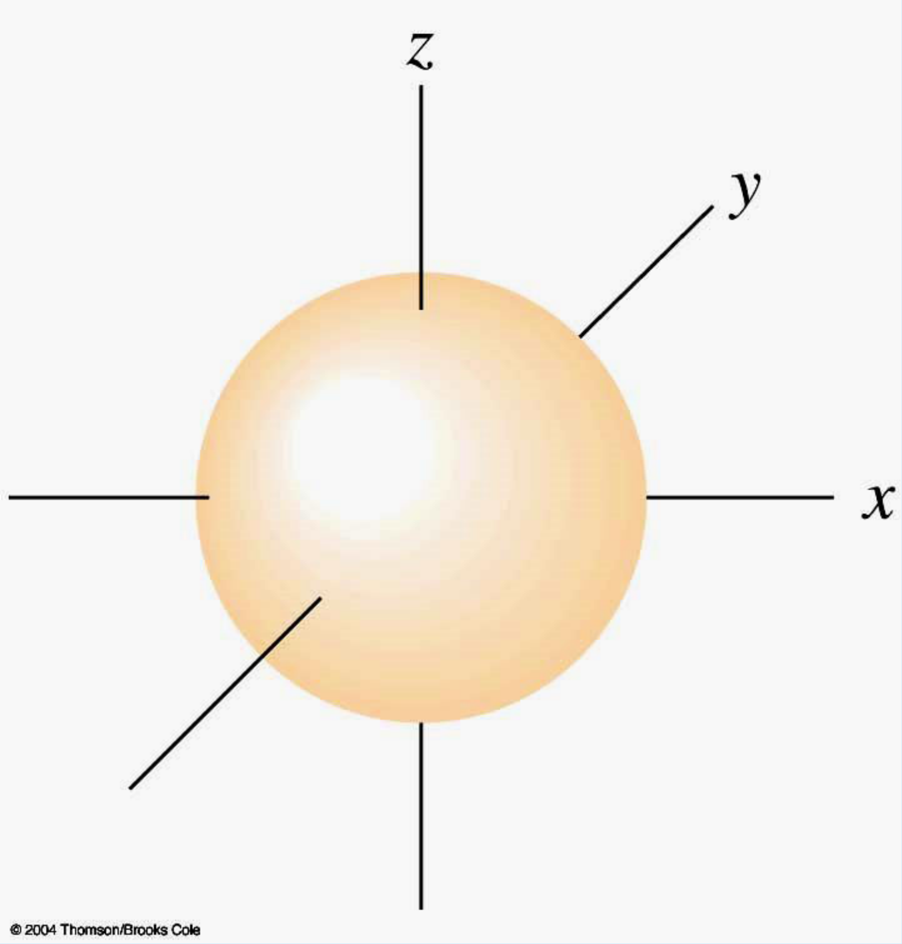
- **PRINCIPAL**: n energy level, distance from nucleus (1, 2, 3, 4…)
- **ANGULAR MOMENTUM**: ℓ shape (s = 0, p = 1, d = 2, f = 3)
- **MAGNETIC**: m_ℓ spatial orientation
  (0 for s; -1, 0, +1 for p; -2, -1, 0, +1, +2 for d, *etc*.)
- **SPIN**: m_s spin ($+{}^{1}/_{2}$ or $-{}^{1}/_{2}$)

- **S orbital properties**:

  There is one s orbital per n level.

  $\ell = 0$ and only one value of $m_\ell = 0$

- **S orbitals are spherically symmetric**

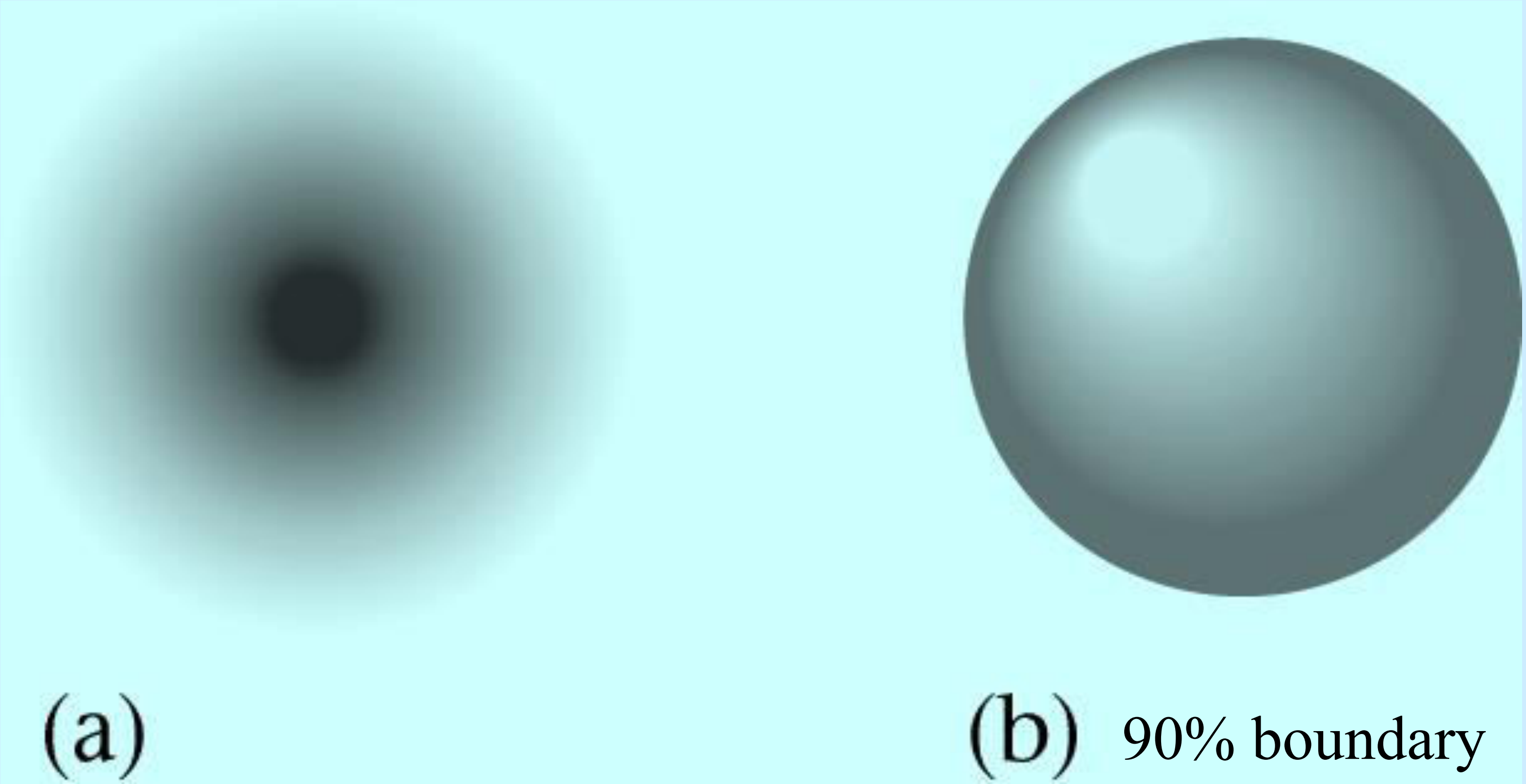


✓ **For every s orbital:**

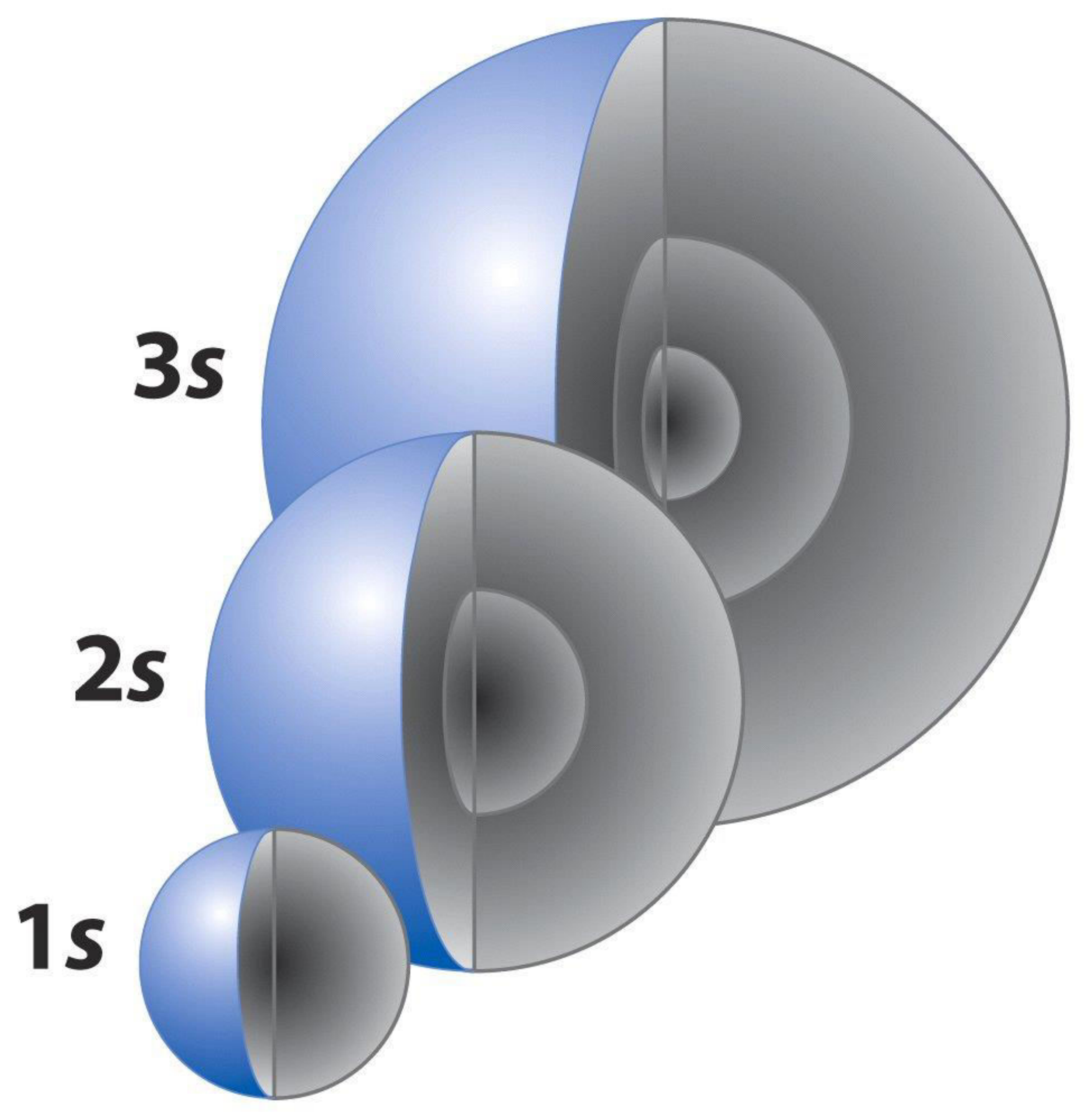
$\ell = 0$ and $m_\ell = 0$

✓ The only thing that changes for s orbitals is n.

- Orbitals do not have sharp boundaries.

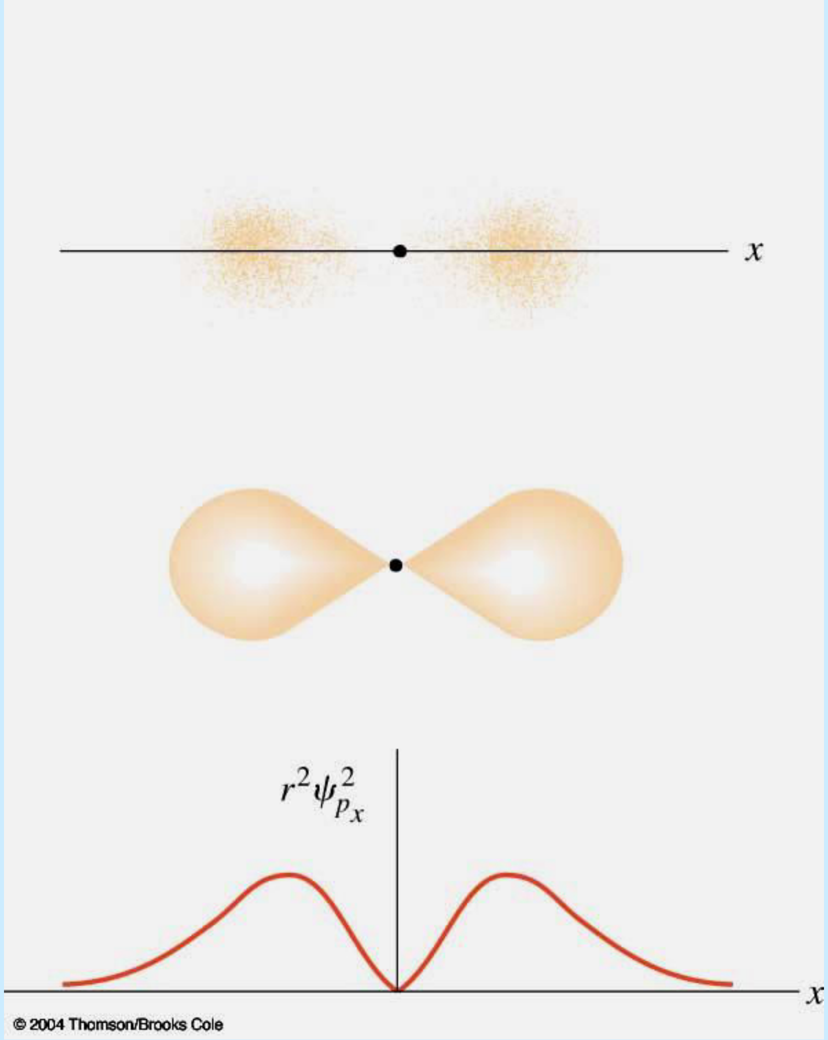


90% boundary



Three dimensional depictions of electron distribution

- p orbitals are peanut or dumbbell shaped.



© 2004 Thomson/Brooks Cole

$\ell = 1$

The first p orbitals appear in the $n = 2$ shell.

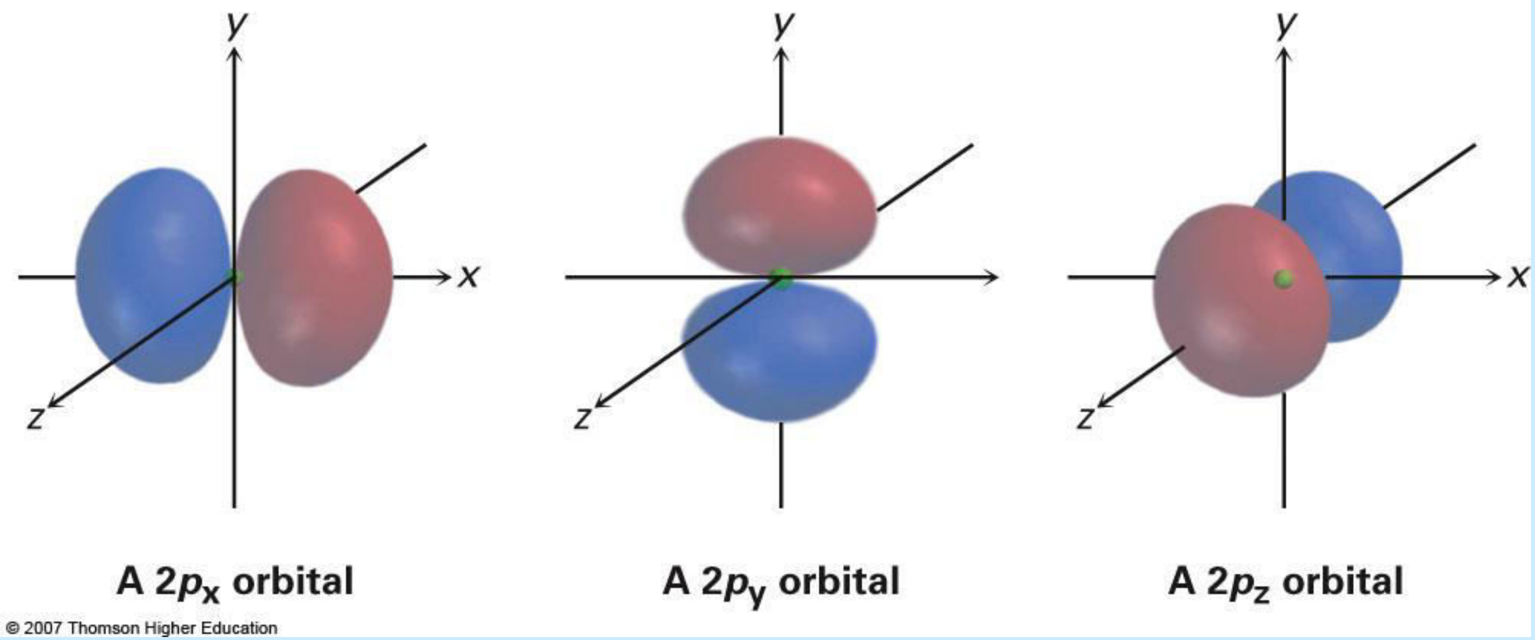
There are 3 p orbitals per n level.
The three orbitals are named
p_x, p_y, p_z.

$\ell = 1$ for all p orbitals.

$m_\ell = -1, 0, +1$ (designate the three orientations)

p-Orbitals

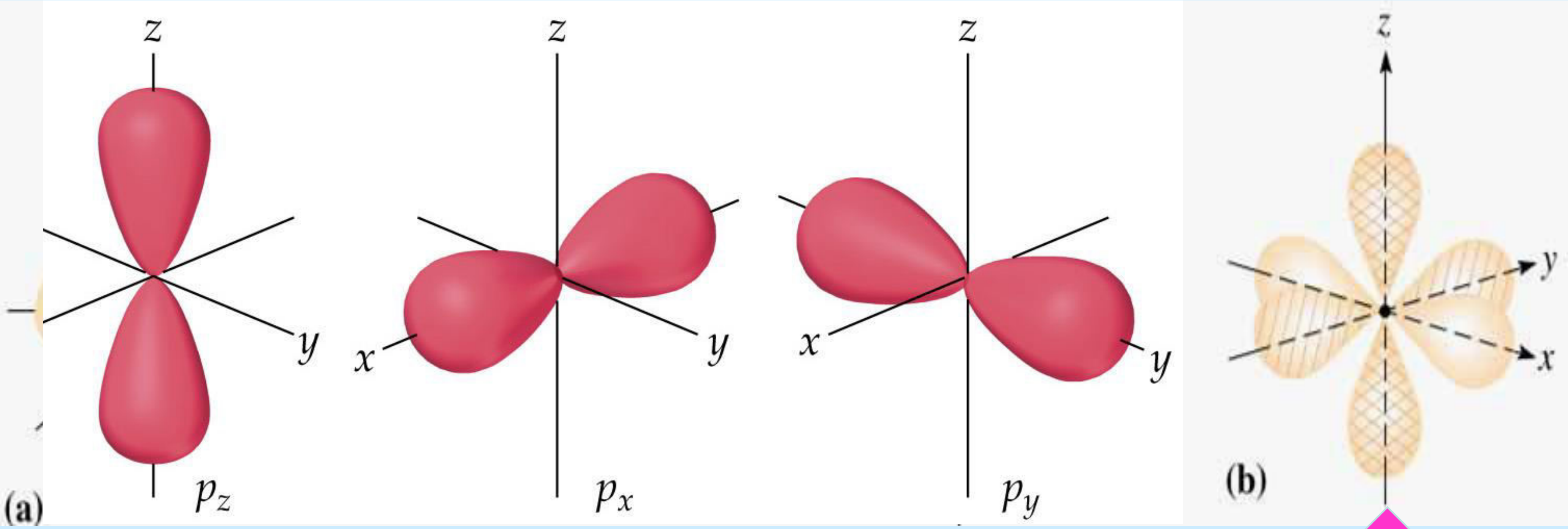
- In each shell there are three perpendicular *p* orbitals, p_x, p_y, and p_z, of equal energy
- Lobes of a *p* orbital are separated by region of zero electron density, a **node**



A 2p_x orbital A 2p_y orbital A 2p_z orbital

- p orbitals are peanut or dumbbell shaped.

$\ell = 1$



$m_\ell = -1, 0, +1$

The three p orbitals and they are perpendicular to each other

d orbital properties:

The first *d* orbitals appear in the n = 3 shell.

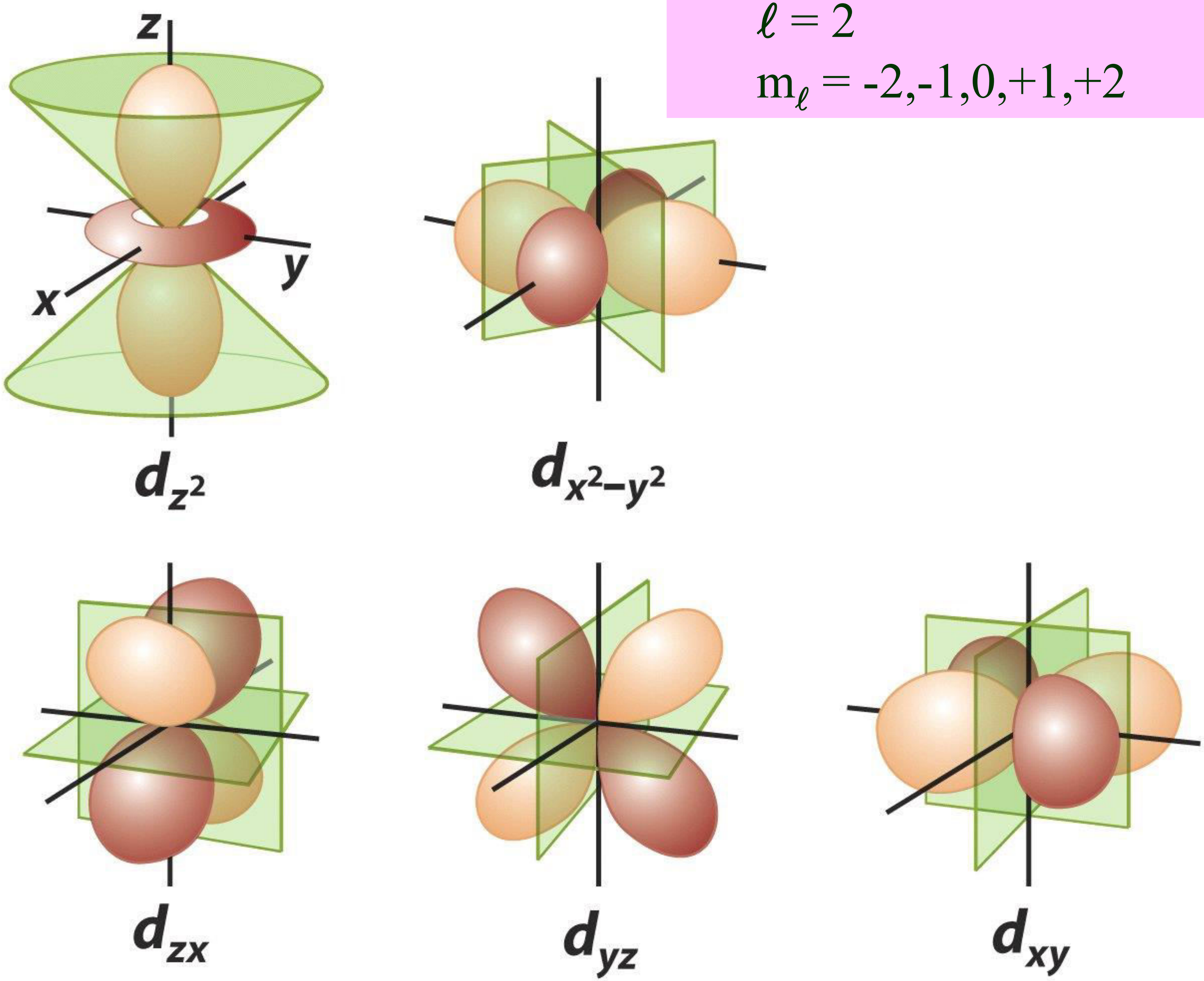
- The five d orbitals have two different shapes:
  - 4 are clover leaf shaped.
  - 1 is peanut shaped with a doughnut around it.
  - The orbitals lie directly on the Cartesian axes or are rotated 45° from the axes.

- There are 5 d orbitals per n level.
  - The five orbitals are named:
  - They have an $\ell = 2$.
  - $m_\ell = -2,-1,0,+1,+2$ (5 values of m_ℓ **ie $2\ell + 1$**)

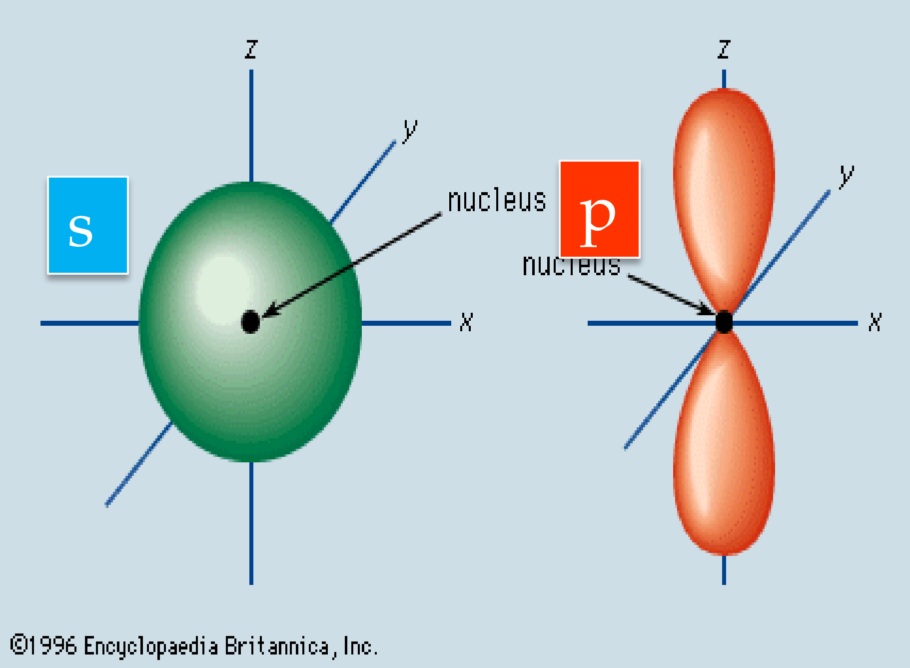
$$d_{xy}, d_{yz}, d_{xz}, d_{x^2-y^2}, d_{z^2}$$

$\ell = 2$

$m_\ell = -2,-1,0,+1,+2$



Orbitals



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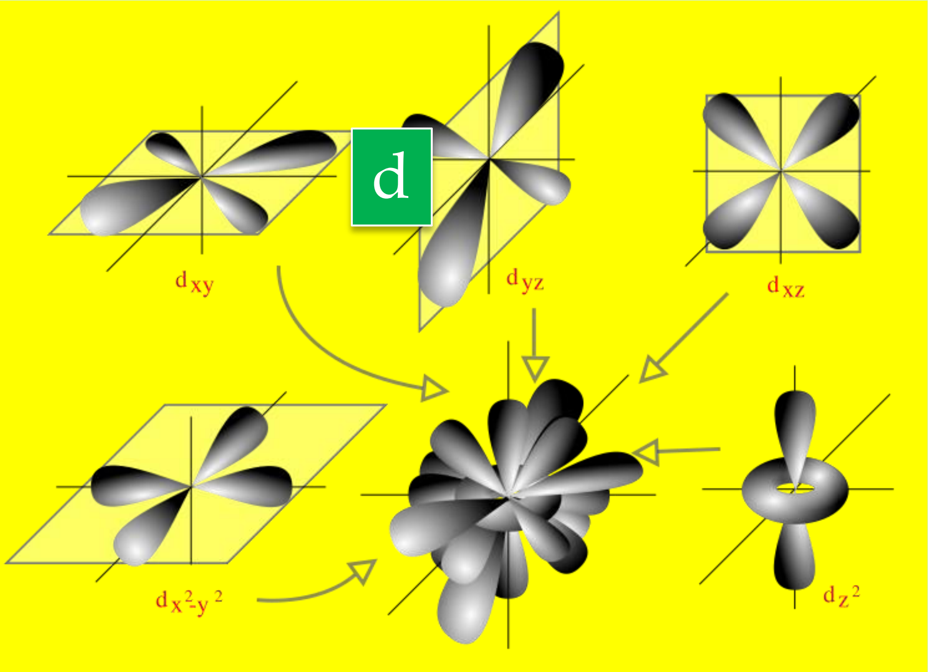


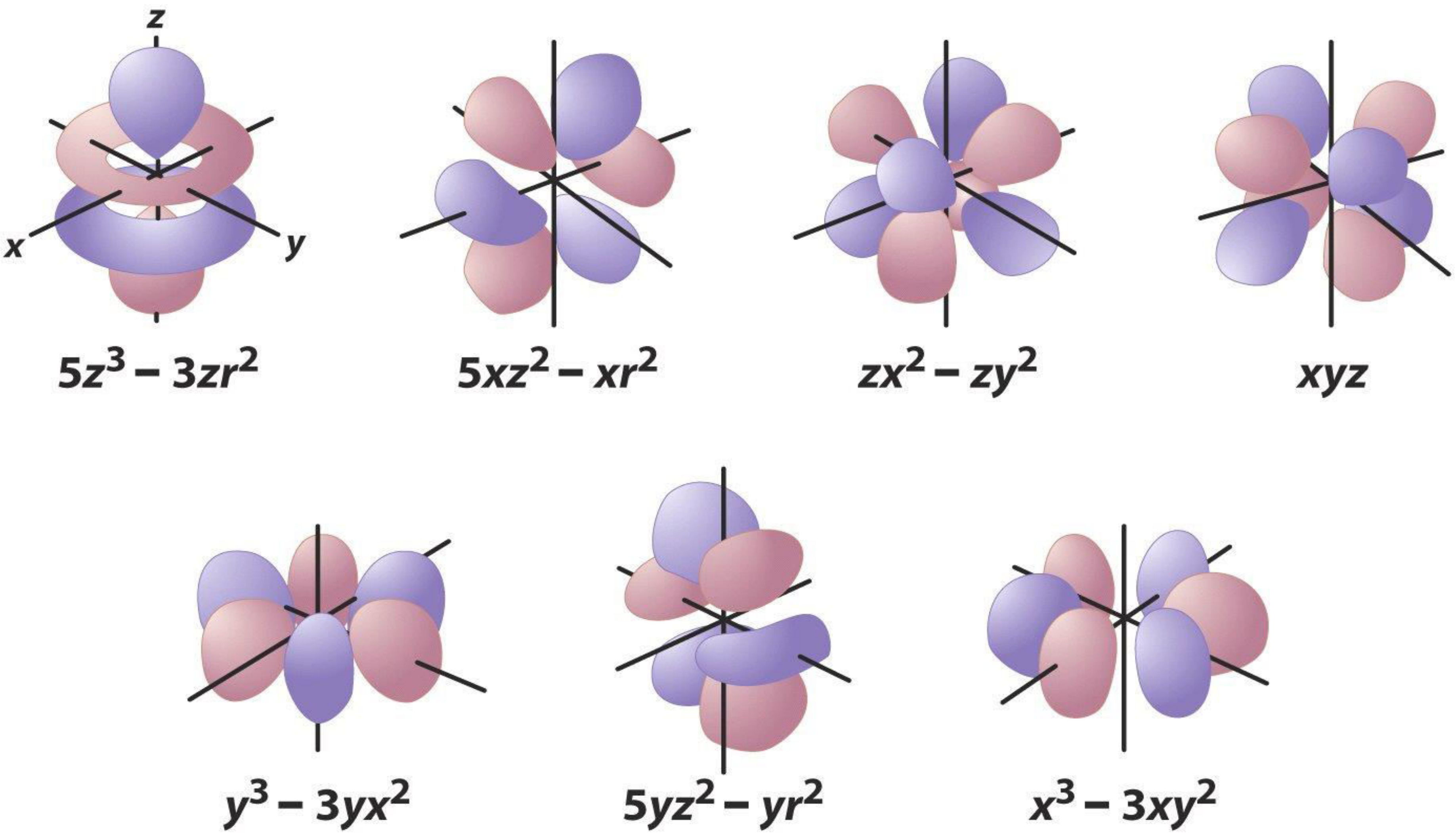
- In the s block, electrons are going into s orbitals.
- In the p block, the s orbitals are full. New electrons are going into the p orbitals.
- In the d block, the s and p orbitals are full. New electrons are going into the d orbitals.
- What about the f block?

f orbital properties:

- The first f orbitals appear in the n = 4 shell.
- The *f* orbitals have the most complex shapes.
- There are seven *f* orbitals per n level.
  - The f orbitals have complicated names.
  - They have an $\ell = 3$
  - m_ℓ = -3,-2,-1,0,+1,+2, +3 7 values

$\ell = 3$

m_ℓ = -3,-2,-1,0,+1,+2, +3 (7 values)



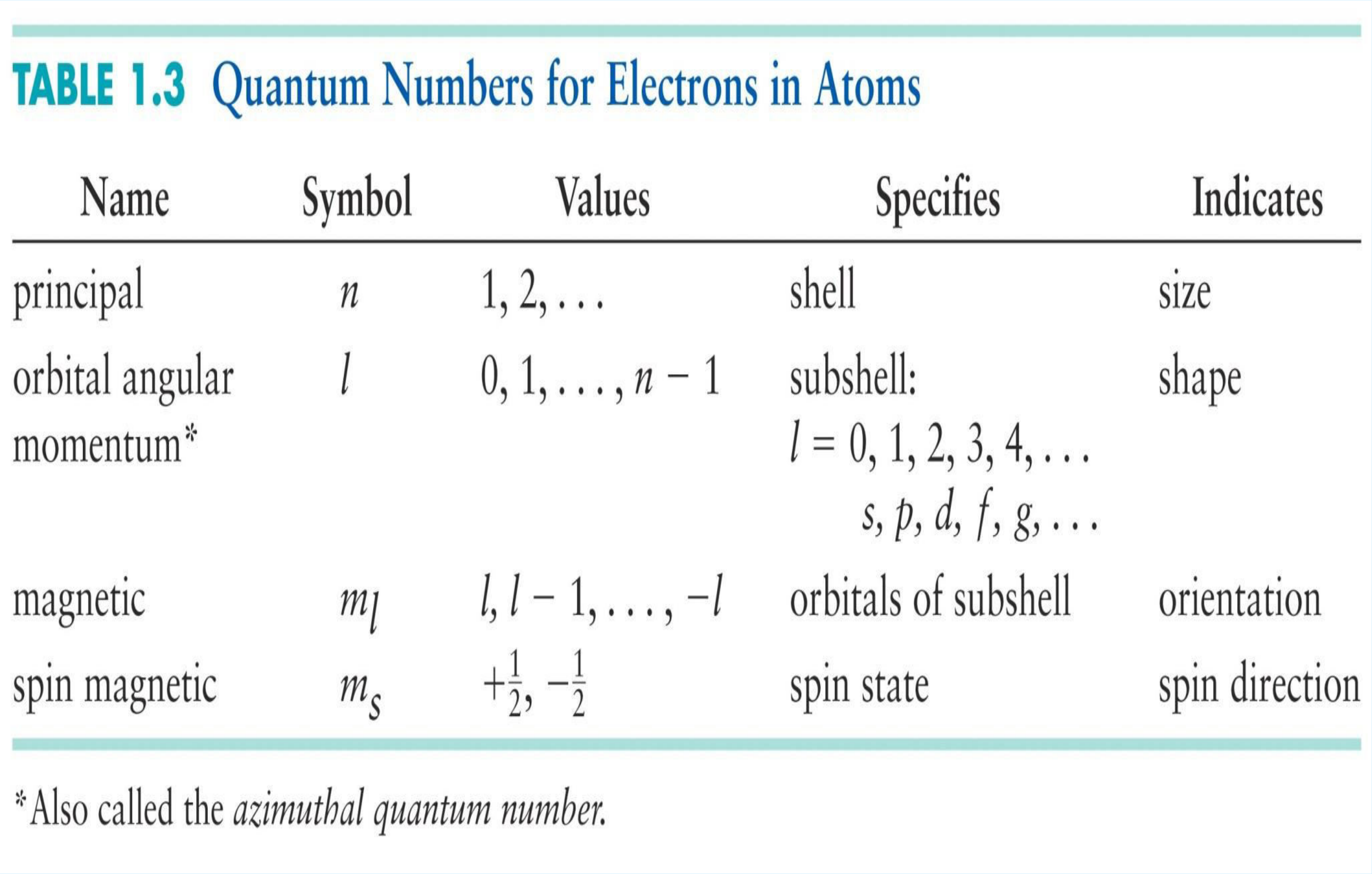
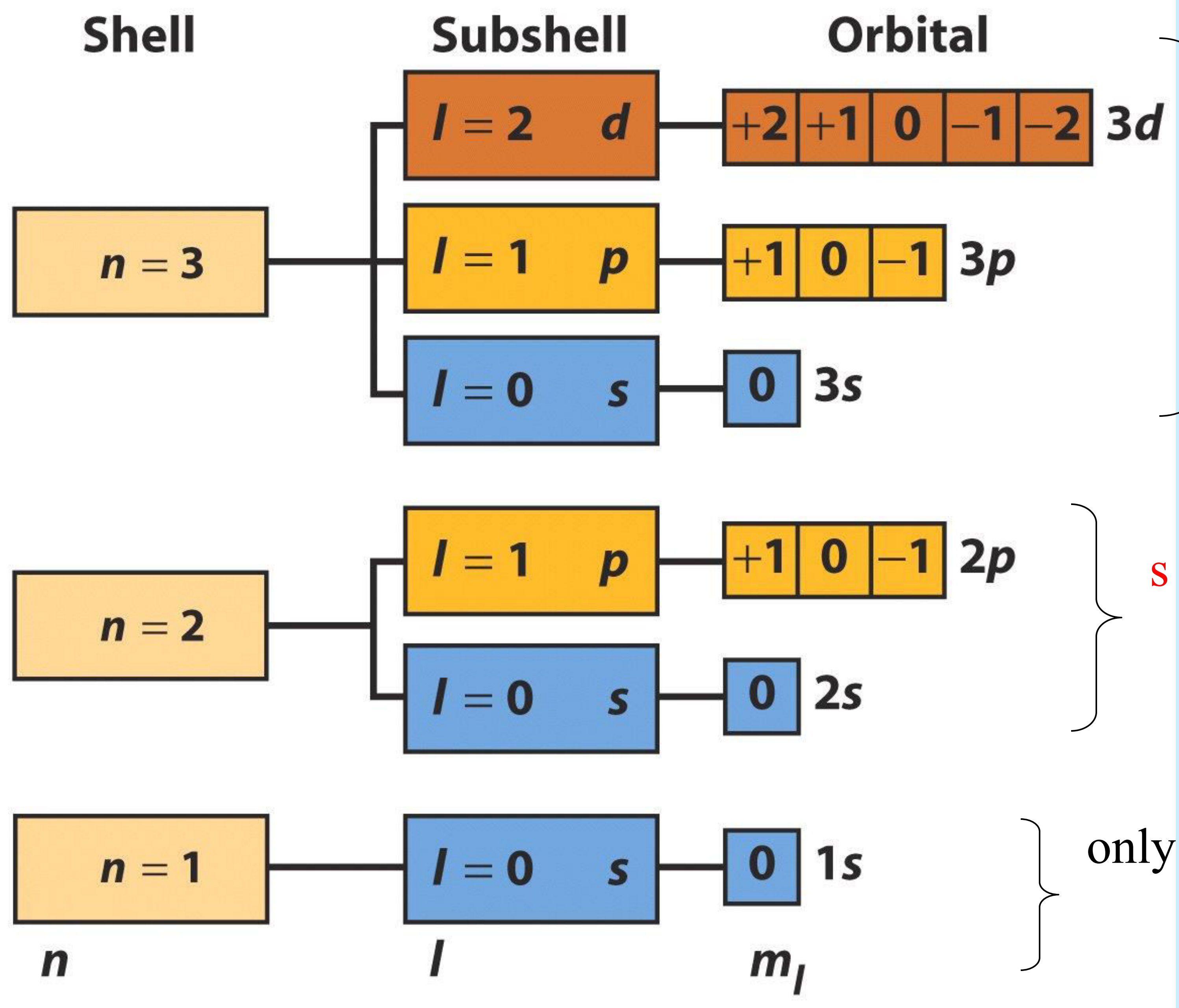


TABLE 1.3 Quantum Numbers for Electrons in Atoms

Name	Symbol	Values	Specifies	Indicates
principal	n	$1, 2, \ldots$	shell	size
orbital angular momentum*	l	$0, 1, \ldots, n-1$	subshell: $l = 0, 1, 2, 3, 4, \ldots$ $s, p, d, f, g, \ldots$	shape
magnetic	m_l	$l, l-1, \ldots, -l$	orbitals of subshell	orientation
spin magnetic	m_s	$+\frac{1}{2}, -\frac{1}{2}$	spin state	spin direction

*Also called the *azimuthal quantum number.*



s, p and d

s and p

only s

- Electron Configurations

Electronic Configurations

- Electronic configuration is the specific way in which the atomic orbitals are filled.

- Think of it as being similar to your address. The electron configuration tells me where all the electrons "live."

Electron Locations

Main Energy Levels	**Sublevels**
n=4	4s, 4p, 4d, 4f (same energy level)
n=3	3s, 3p, 3d
n=2	2s, 2p
n=1	1s

Electrons Allowed

- All electrons in the same sublevel have the same energy.

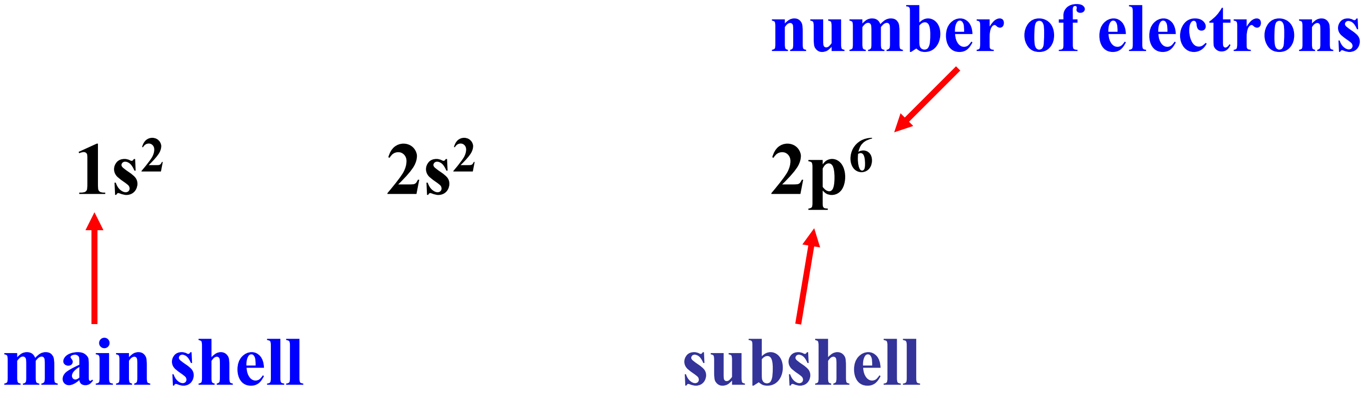
- All 2s electrons have the same energy. All 2p electrons have the same energy which is slightly higher than the energy of the 2s electrons

s sublevel	2 electrons
p sublevel	6 electrons
d sublevel	10 electrons
f sublevel	14 electrons

Electron Configuration

- List of subshells containing electrons
- Written in order of increasing energy
- Superscripts give the number of electrons

Example: Electron configuration of neon (10 e)



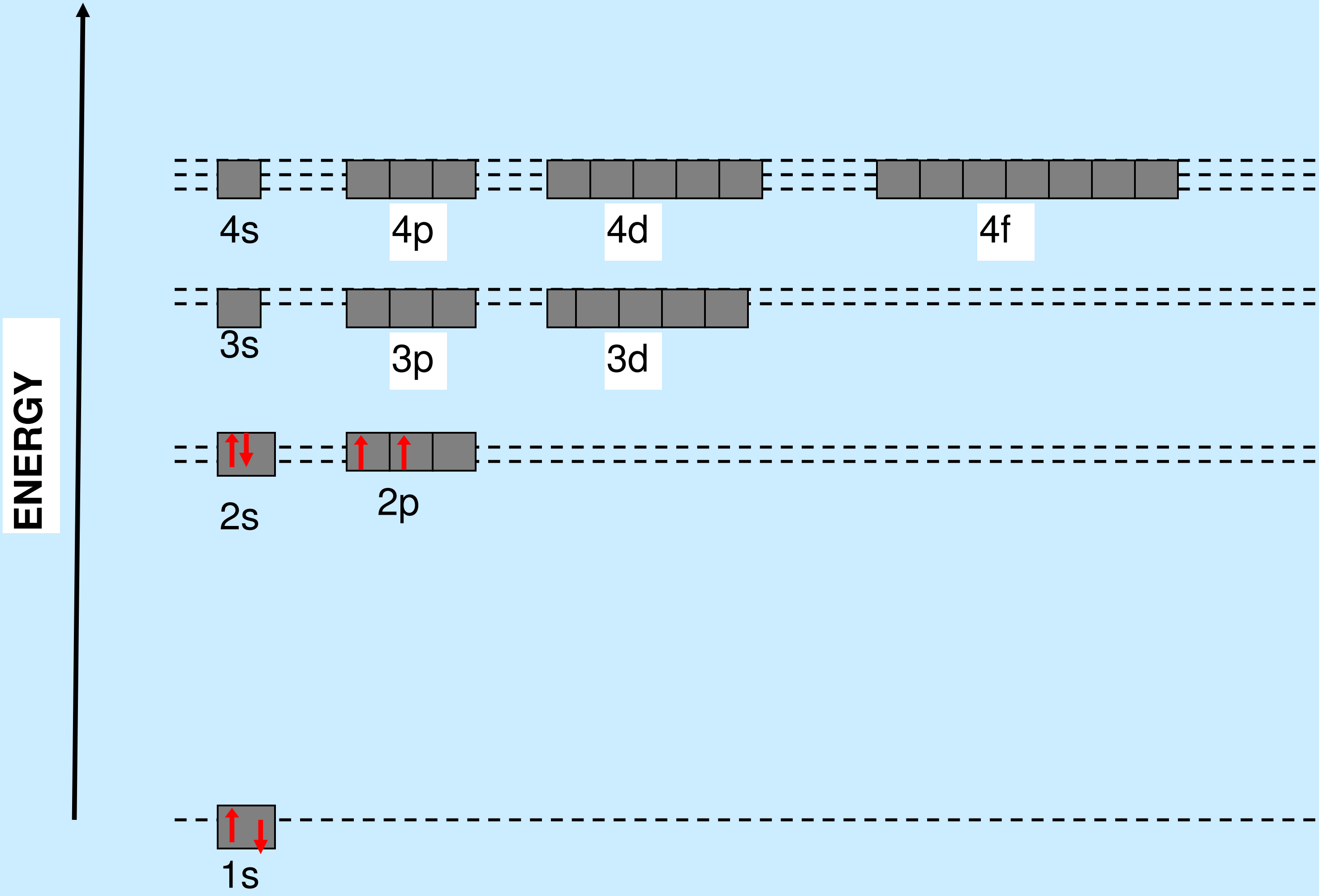
number of electrons

$1s^2$ $2s^2$ $2p^6$

main shell

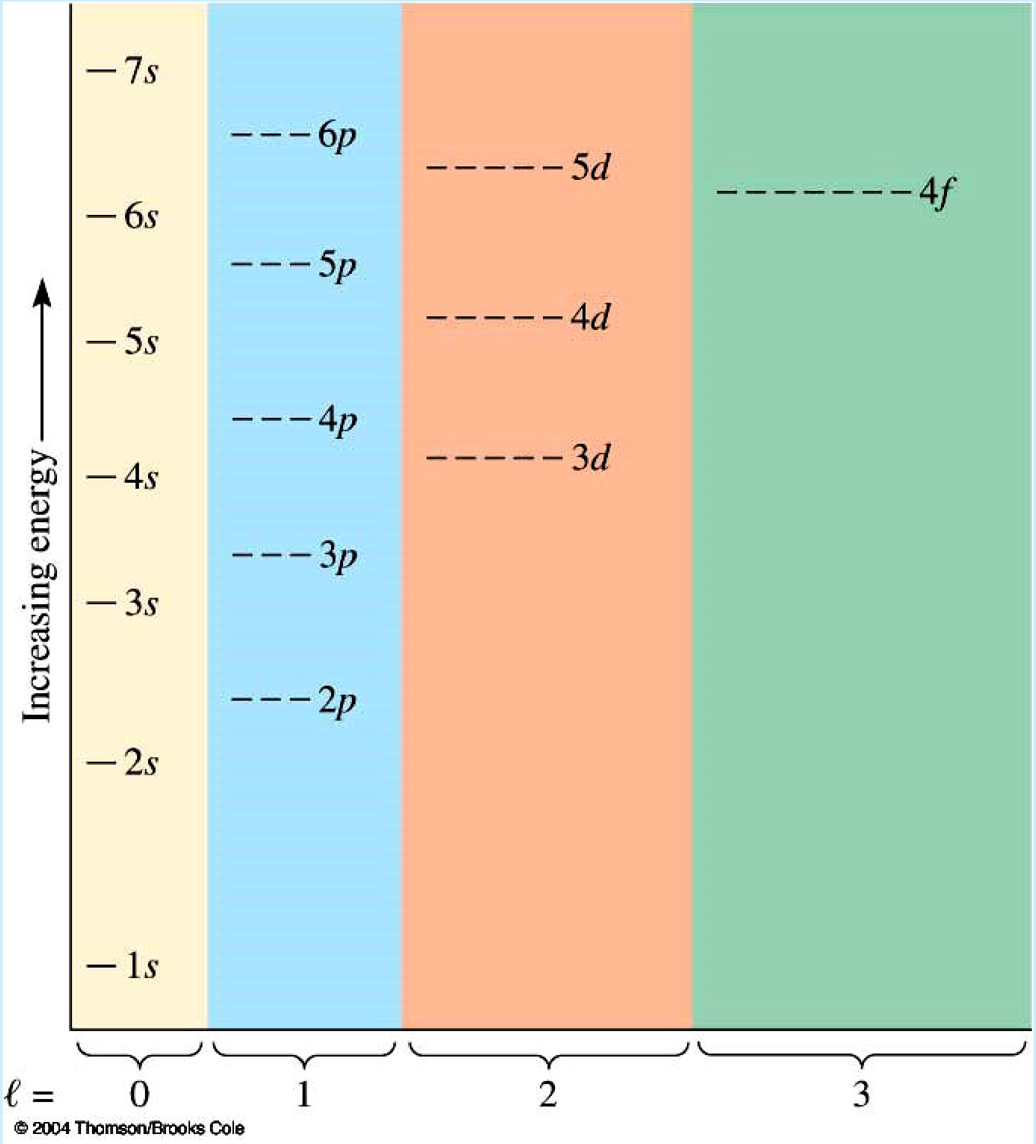
subshell

Orbital Energy Diagram for Carbon



Energy levels of the various atomic orbitals are dictated by Attraction by nucleus only.

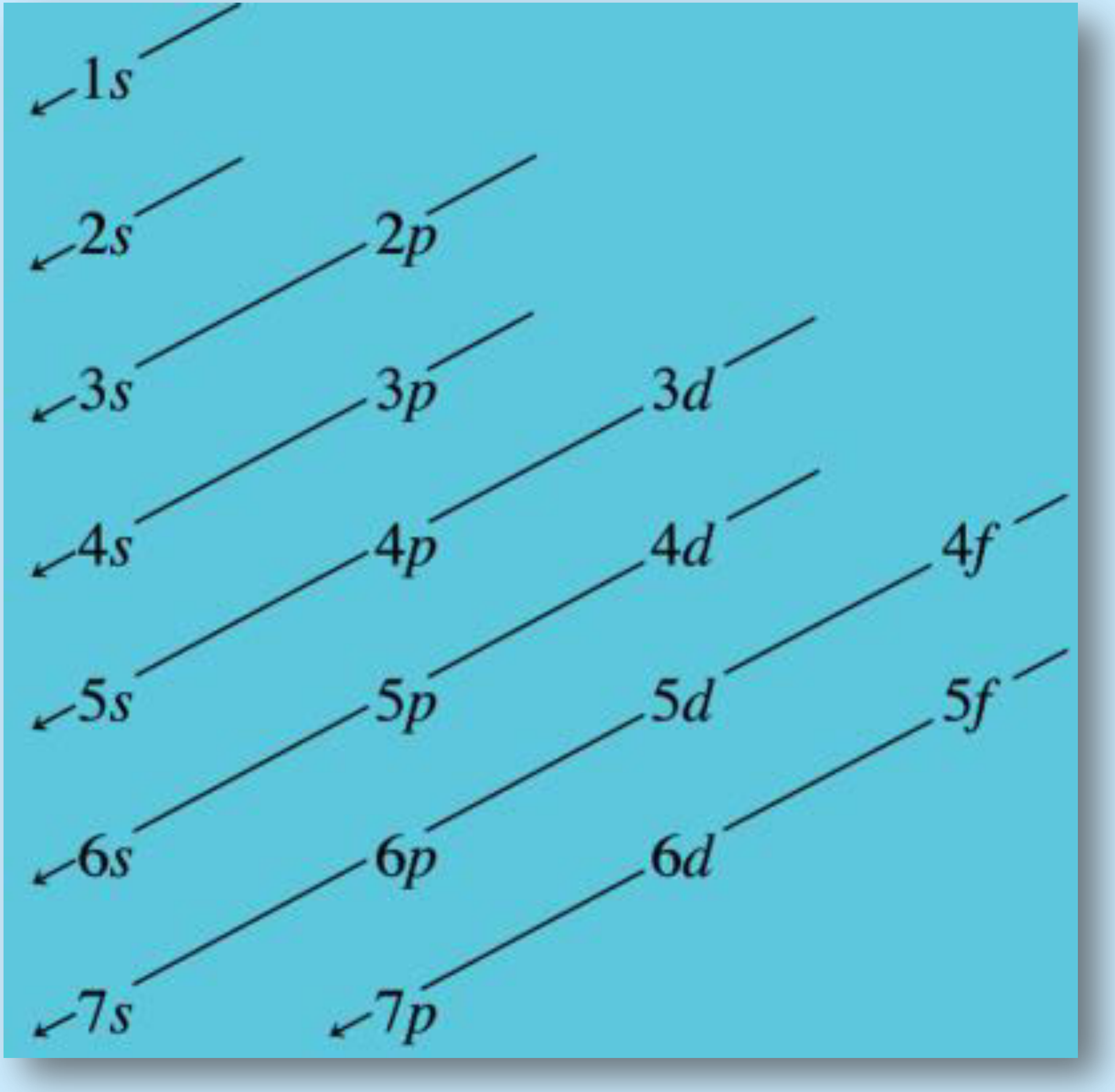
- The **Aufbau Principle** describes the electron filling order in atoms.



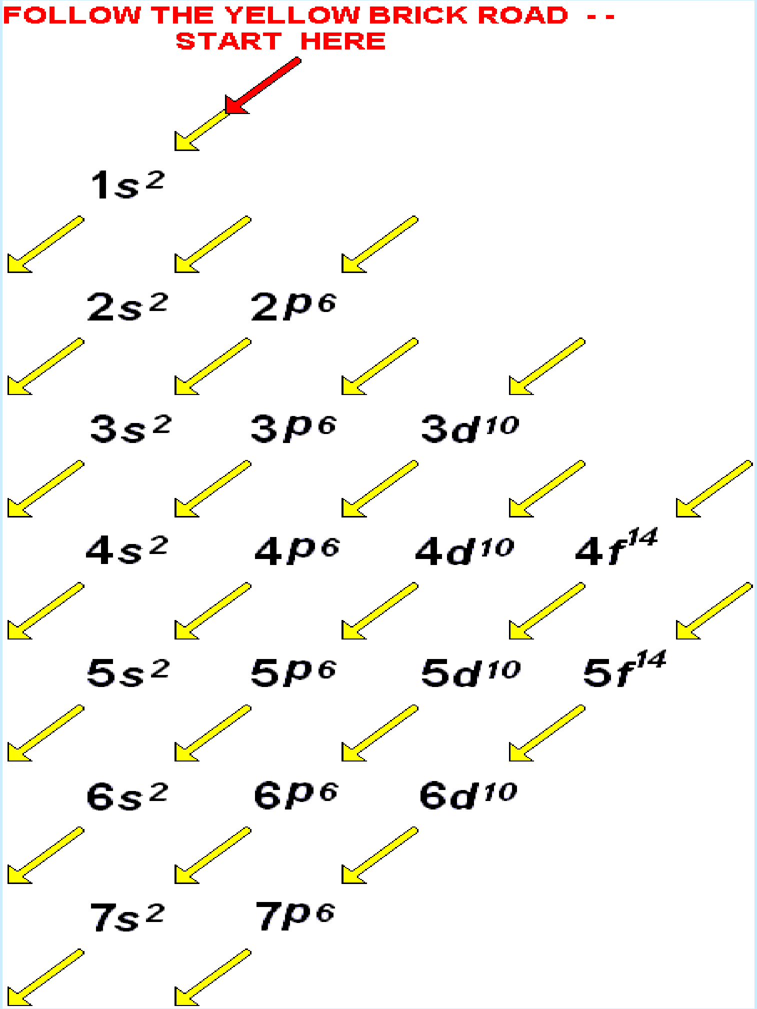
Energy levels of the various atomic orbitals appear somehow distorted due to:

1. Attraction by nucleus
2. Repulsion effect among the electrons
3. Shielding effect of electrons from nucleus attraction

The **Aufbau Principle** describes the electron filling order in atoms.



Rules for Electron Configurations



FOLLOW THE YELLOW BRICK ROAD - -
START HERE

$1s^2$

$2s^2$ $2p^6$

$3s^2$ $3p^6$ $3d^{10}$

$4s^2$ $4p^6$ $4d^{10}$ $4f^{14}$

$5s^2$ $5p^6$ $5d^{10}$ $5f^{14}$

$6s^2$ $6p^6$ $6d^{10}$

$7s^2$ $7p^6$

- In order to write an electron configuration, we need to know the RULES.
- **3 rules govern electron configurations.**
  - **Aufbau Principle**
  - **Pauli Exclusion Principle**
  - **Hund's Rule**
- Using the orbital filling diagram:

  Start with the 1s orbital. Fill each orbital completely and then go to the next one, until all of the elements have been accounted for.

Pauli Exclusion Principle

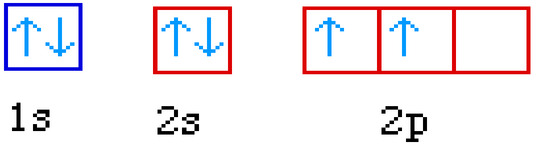
No more than 2 Electrons in Any Orbital…ever.

- The next rule is the Pauli Exclusion Principal.
- **The Pauli Exclusion Principle states that an atomic orbital may have up to 2 electrons and then it is full.**
- The spins have to be paired.
- We usually represent this with an up arrow and a down arrow.
- Since there is only 1 s orbital per energy level, only 2 electrons fill that orbital.

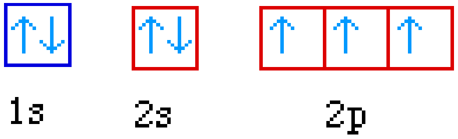
Wolfgang Pauli (a German) - Nobel Prize winner

No two electrons in an atom can have the same set of 4 quantum numbers.

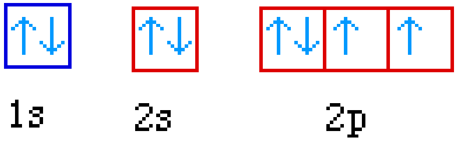
Hund’s Rule



Orbital diagram for carbon



Orbital diagram for nitrogen

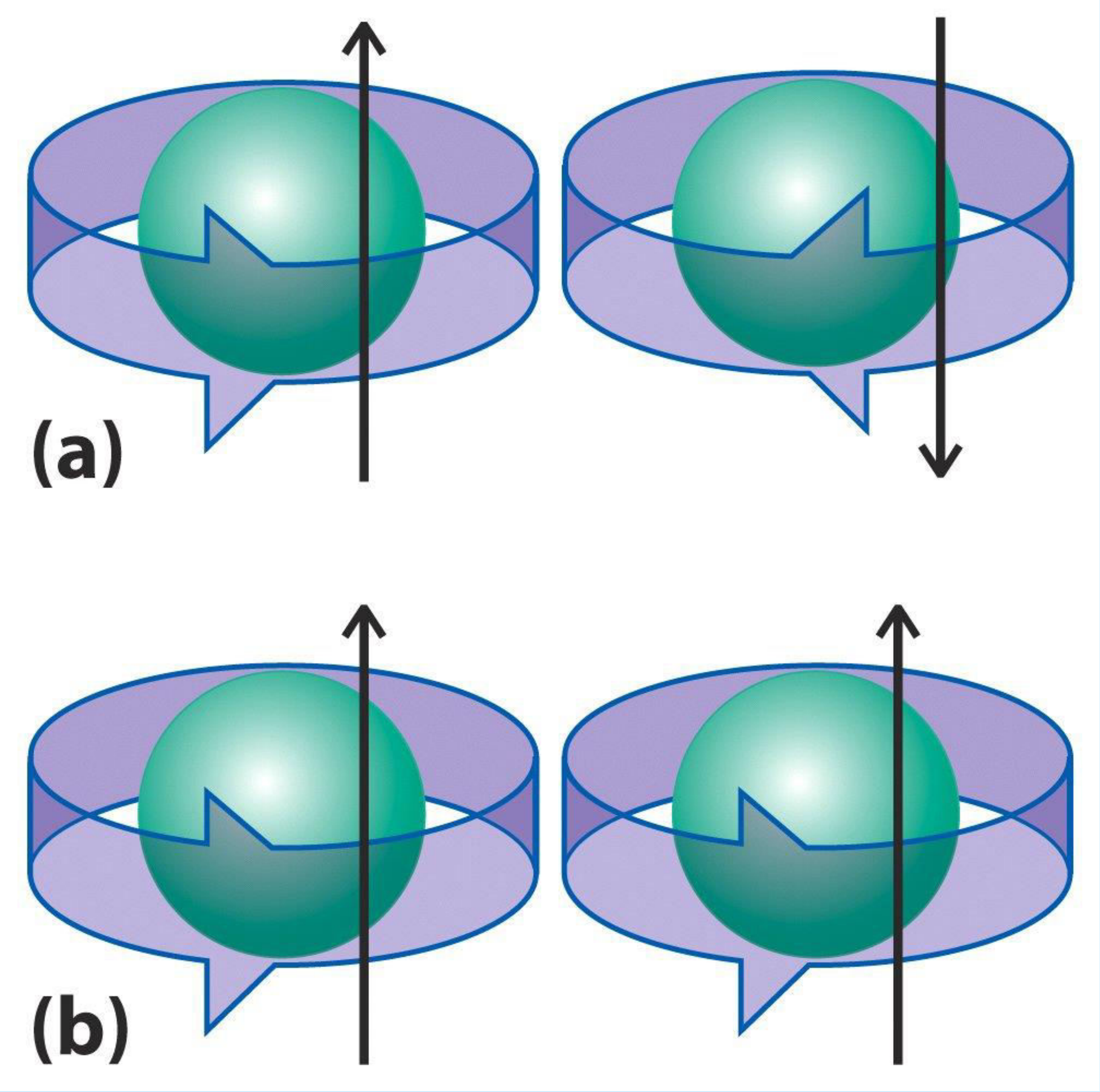


Orbital diagram for oxygen

Don’t pair up the 2p electrons until all 3 orbitals are half full.

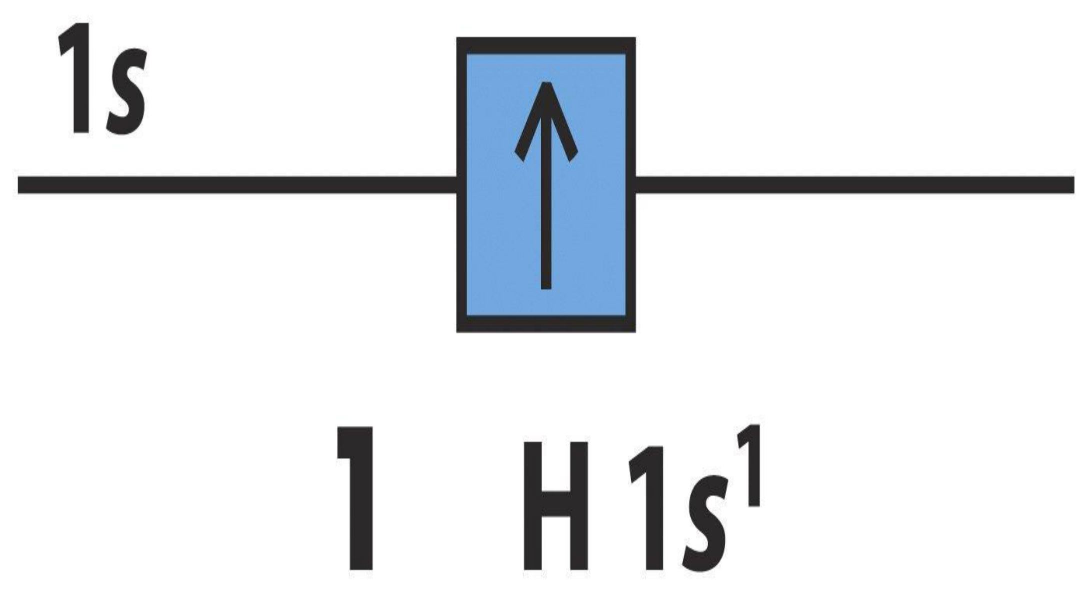
- **Hund’s Rule states that when you get to degenerate orbitals, you fill them all half way first, before you start pairing up the electrons.**

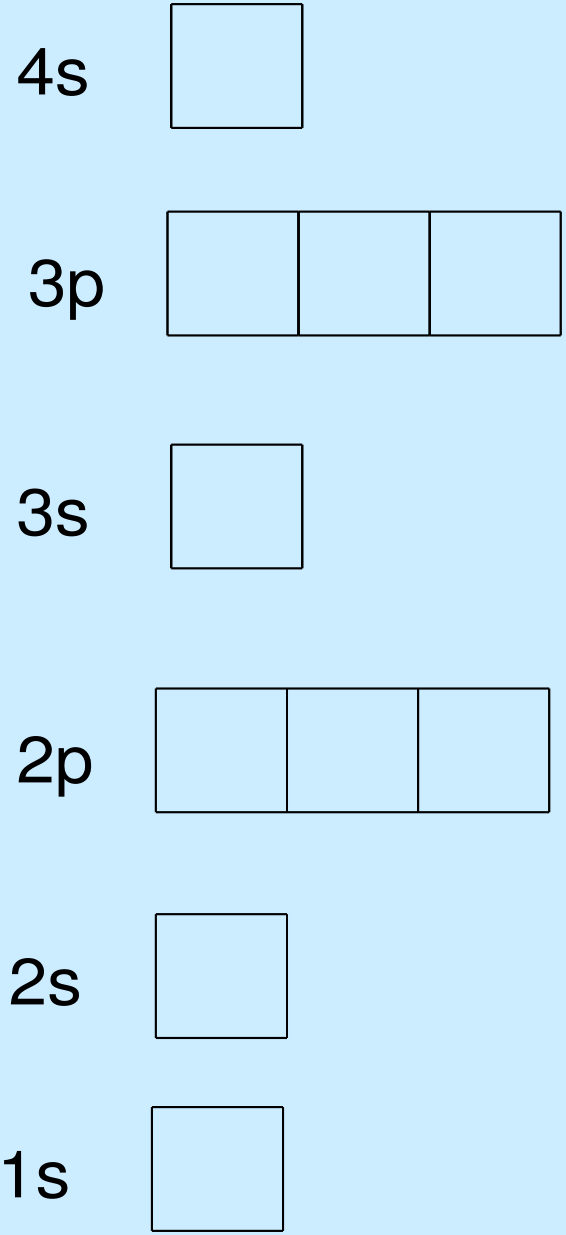
- What are degenerate orbitals?
- Degenerate means they have the same energy.
- So, the 3 p orbitals on each level are degenerate, because they all have the same energy.
- Similarly, the d and f orbitals are degenerate too.



paired

parallel spins




4s

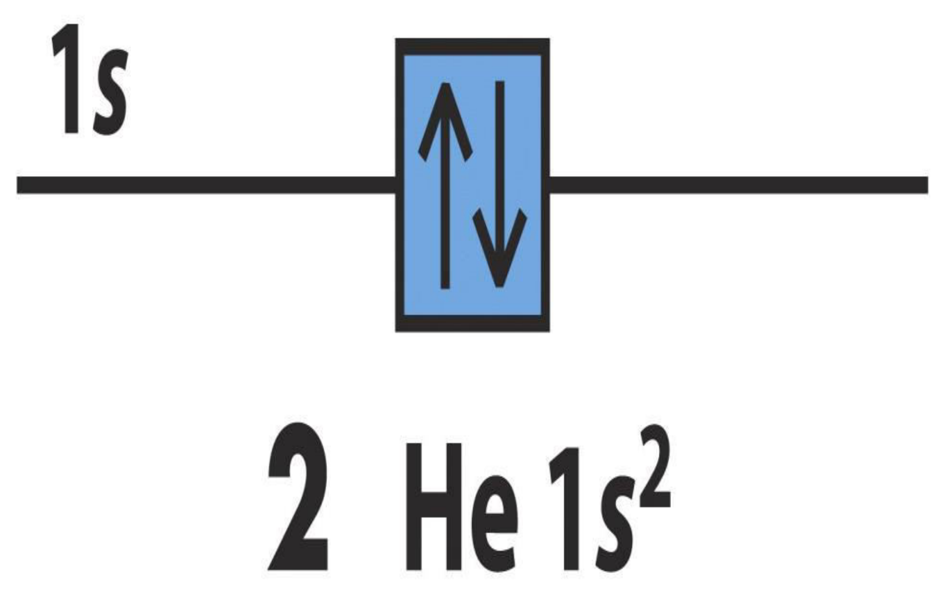
3p

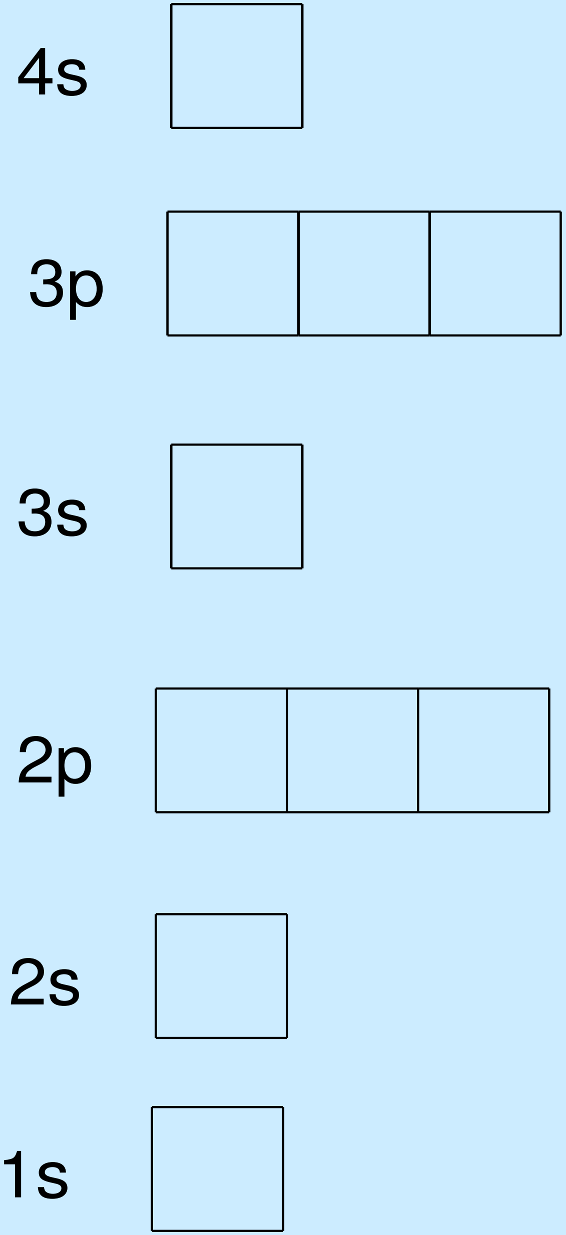
3s

2p

2s

1s




4s

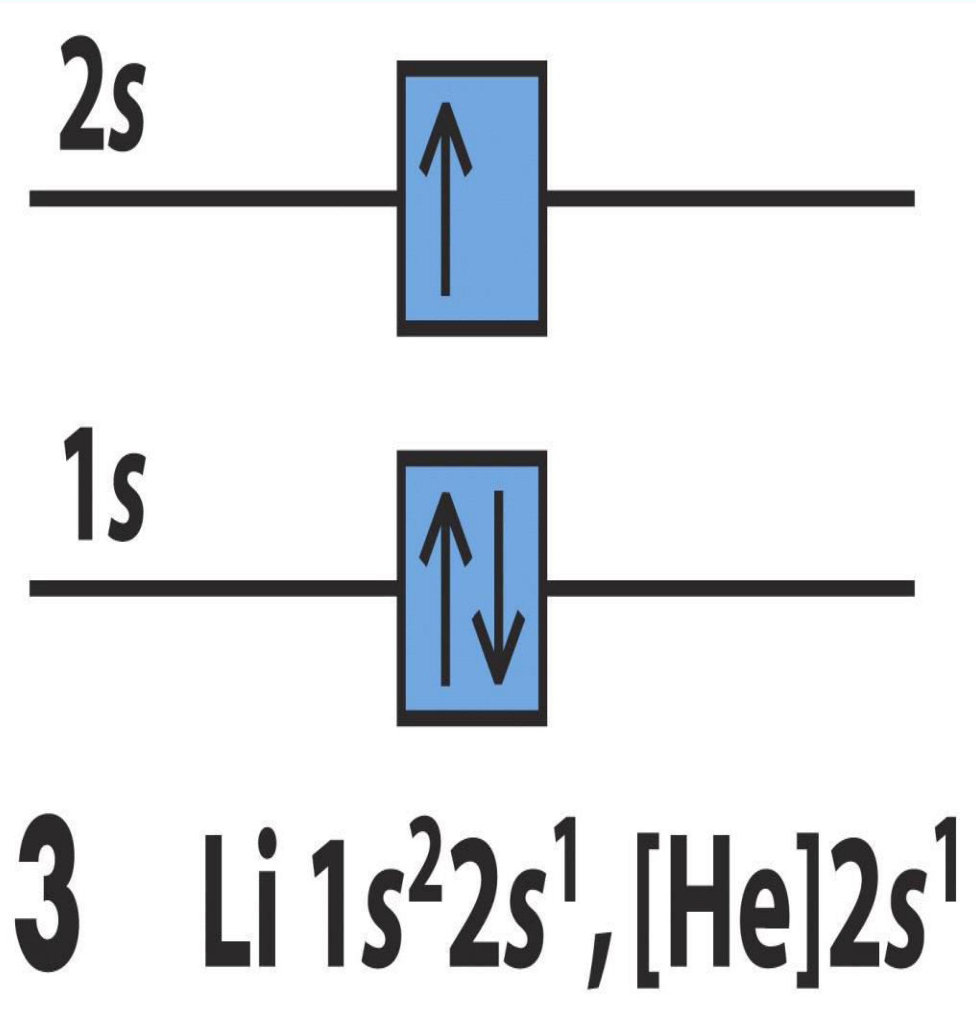
3p

3s

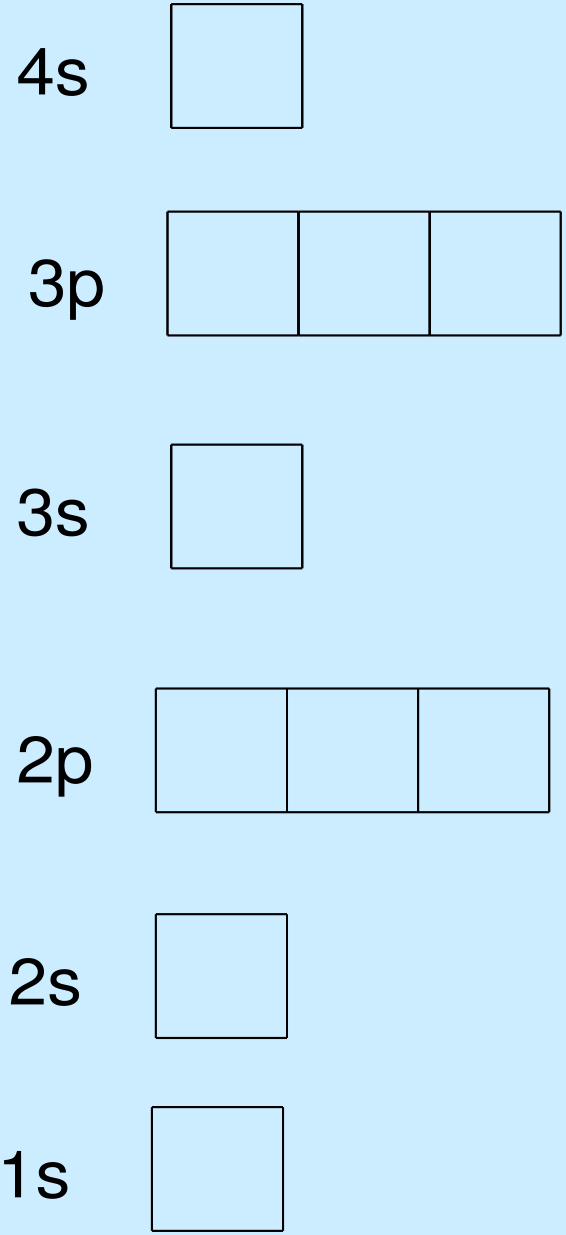
2p

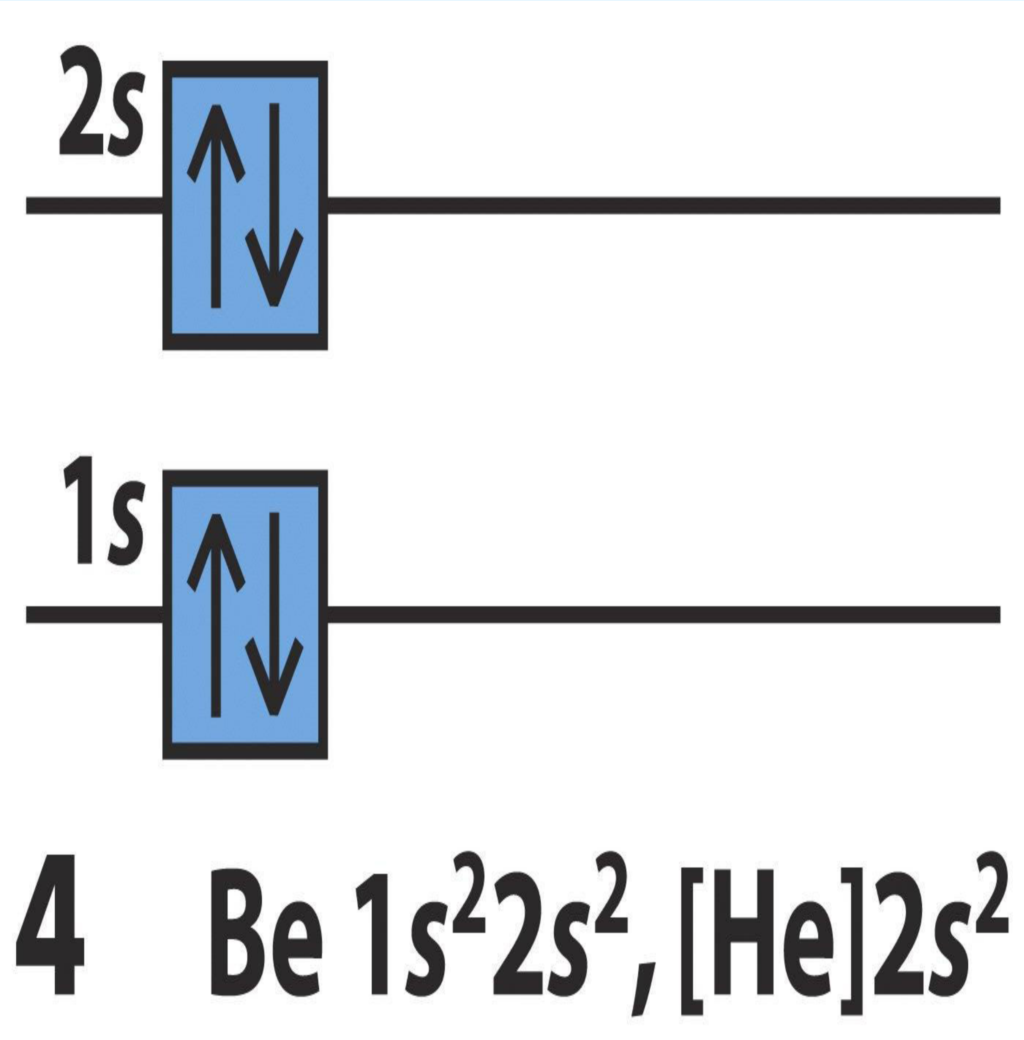
2s

1s

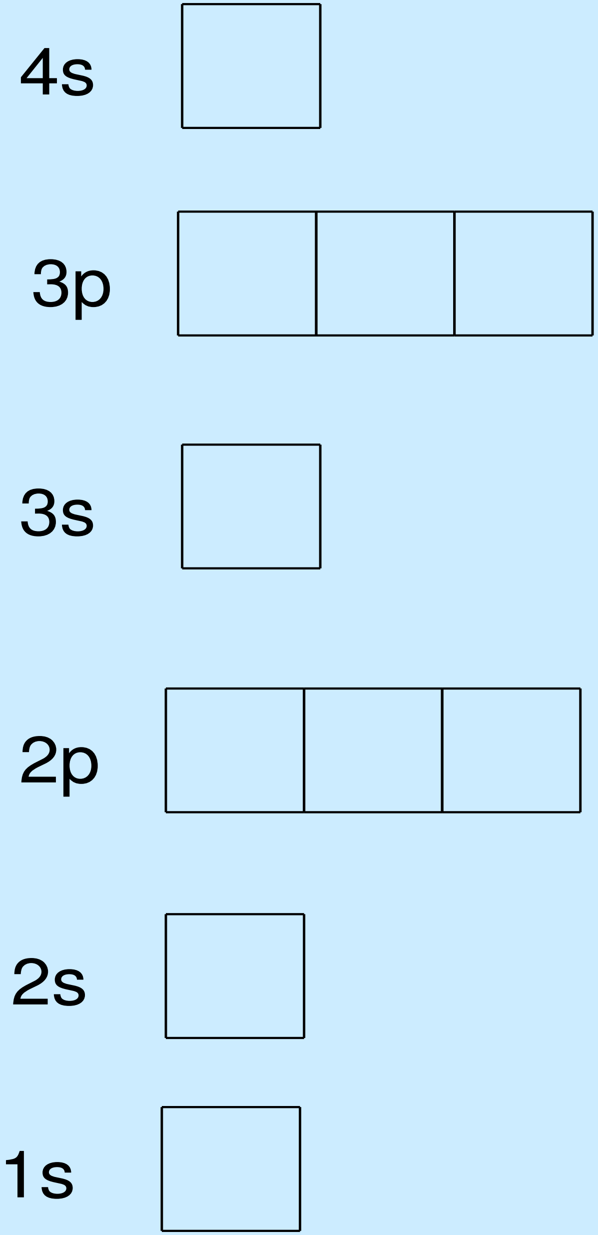


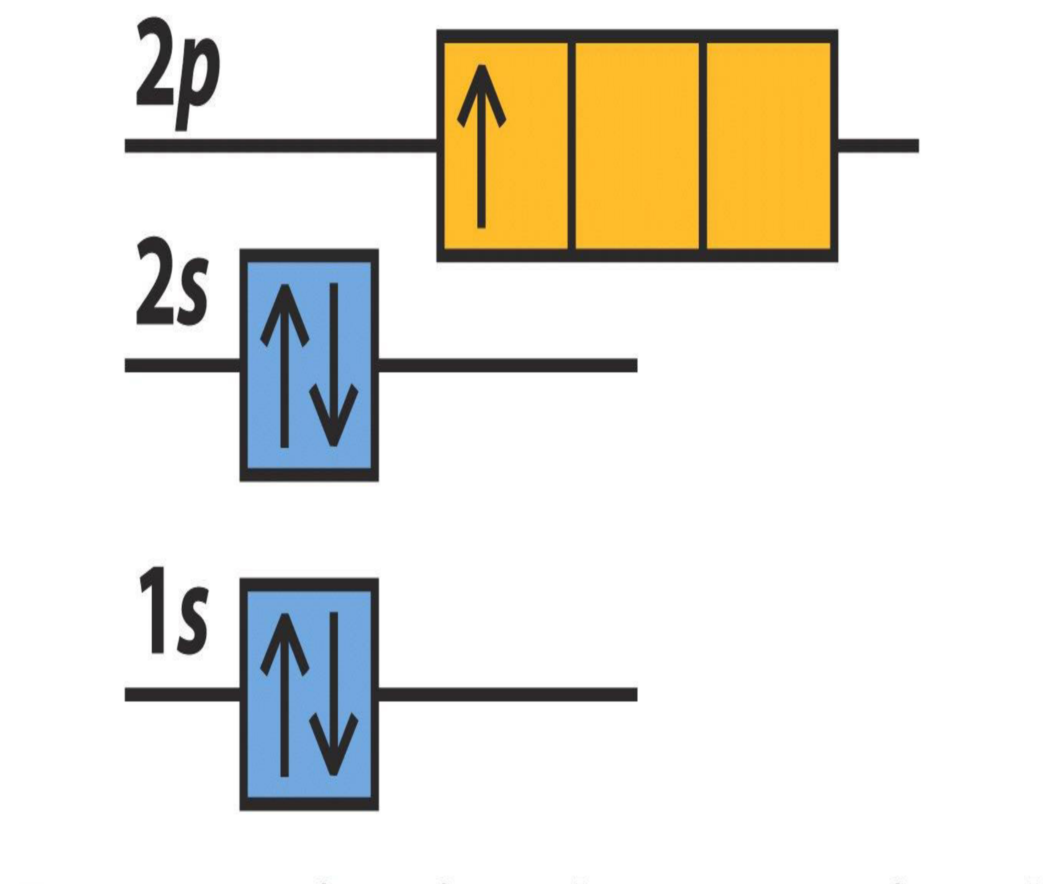
3 Li $1s^2 2s^1$, [He]$2s^1$



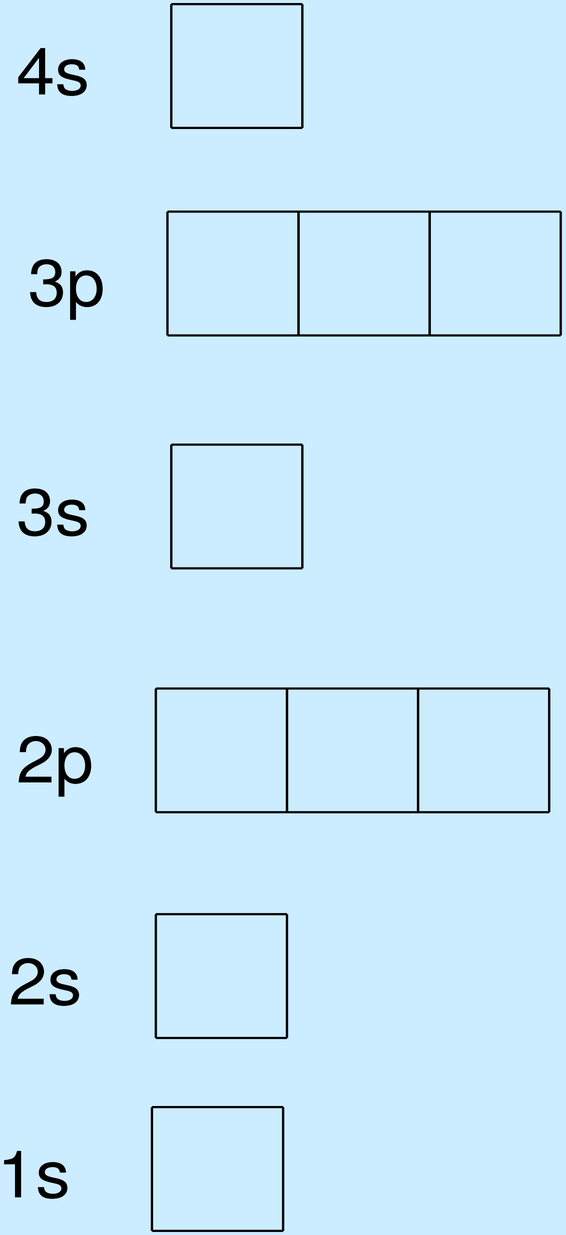


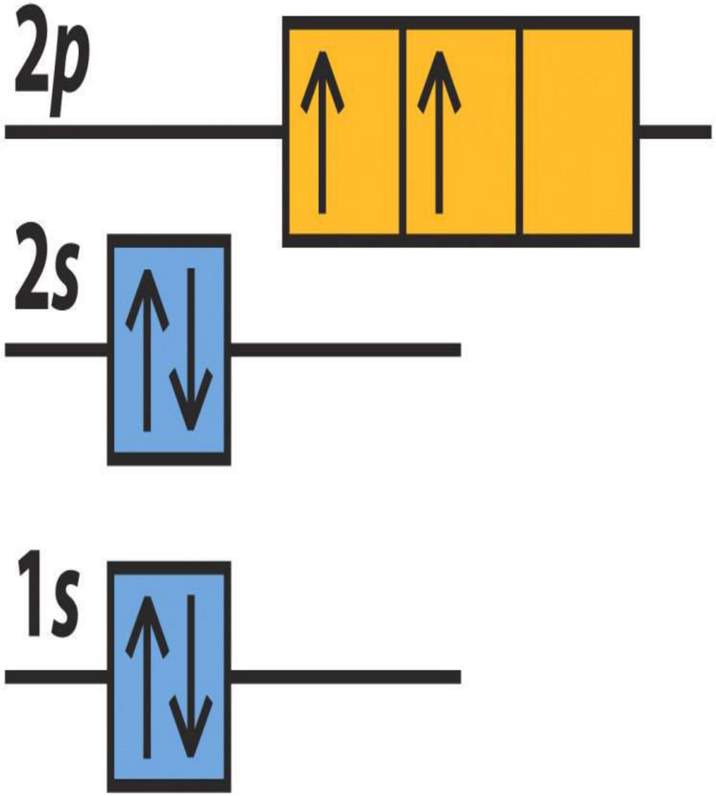
4 Be $1s^2 2s^2$, [He]$2s^2$



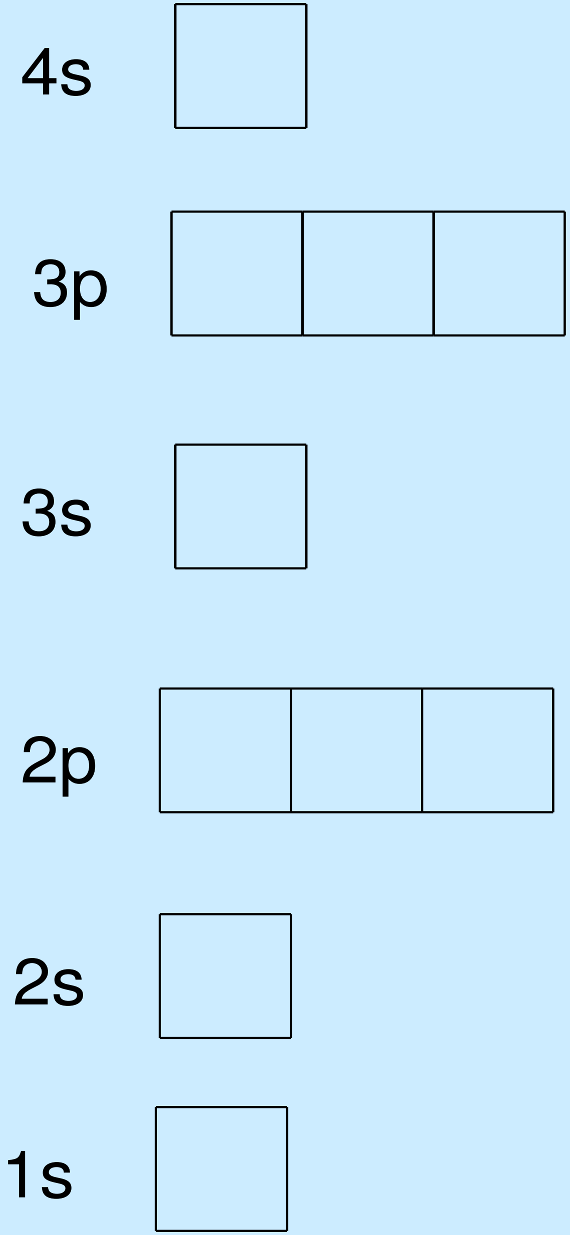


5 B $1s^2 2s^2 2p^1$, [He]$2s^2 2p^1$





6 C $1s^2 2s^2 2p^2$, [He]$2s^2 2p^2$

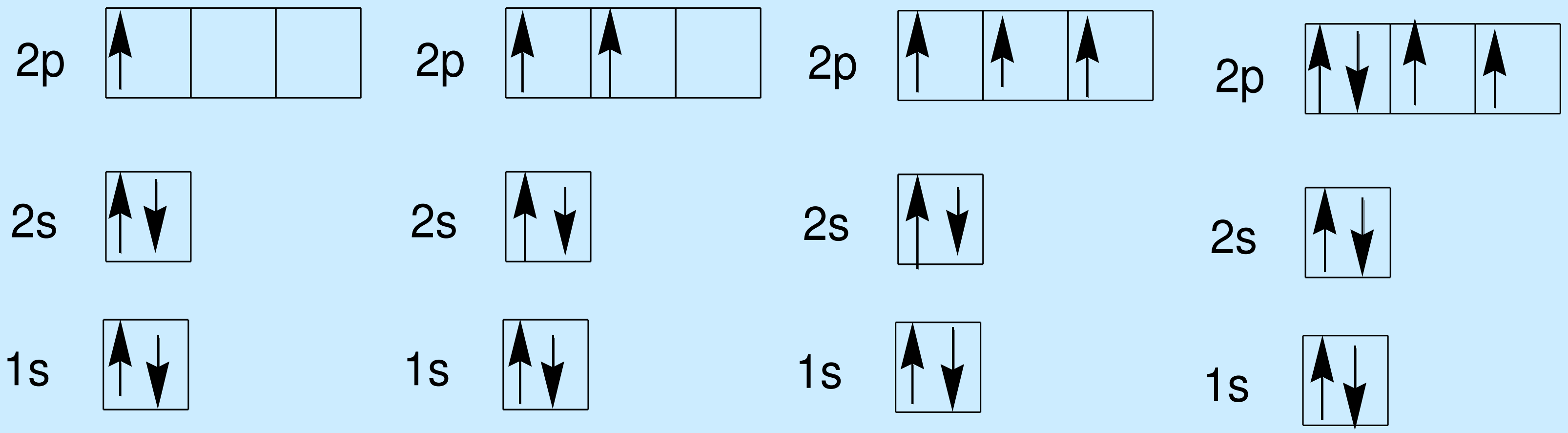


The order of orbital levels is:

1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d 6p 7s …..

Know configurations up to Ba!

Electron Configurations

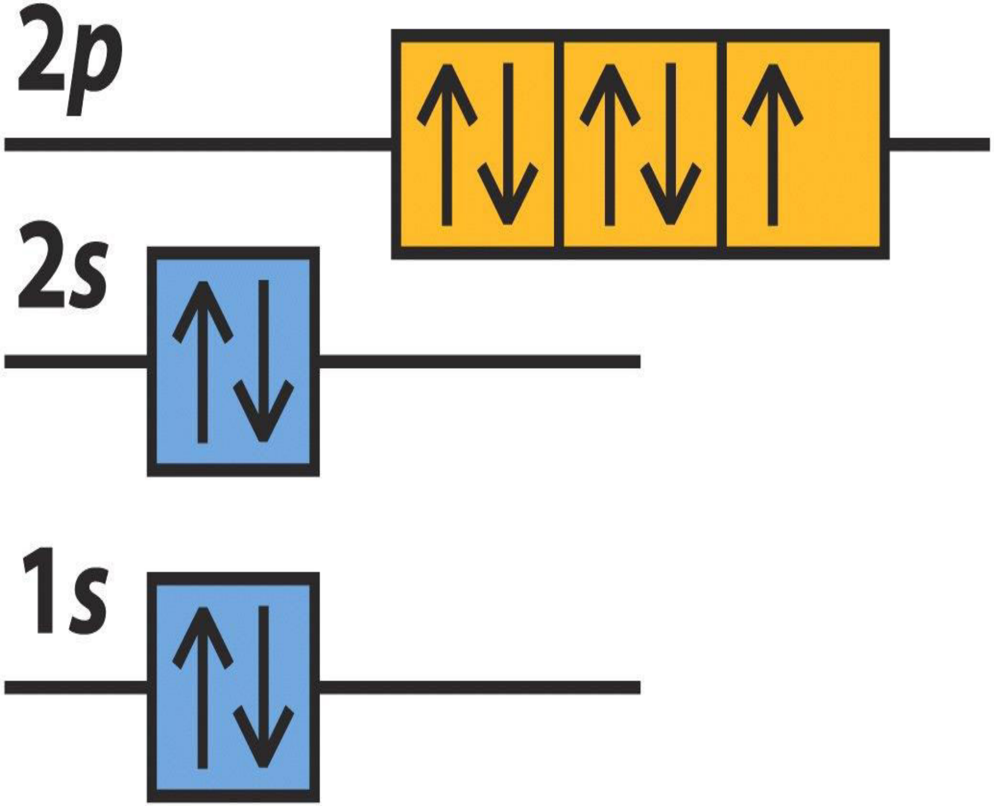


2p 2p 2p 2p

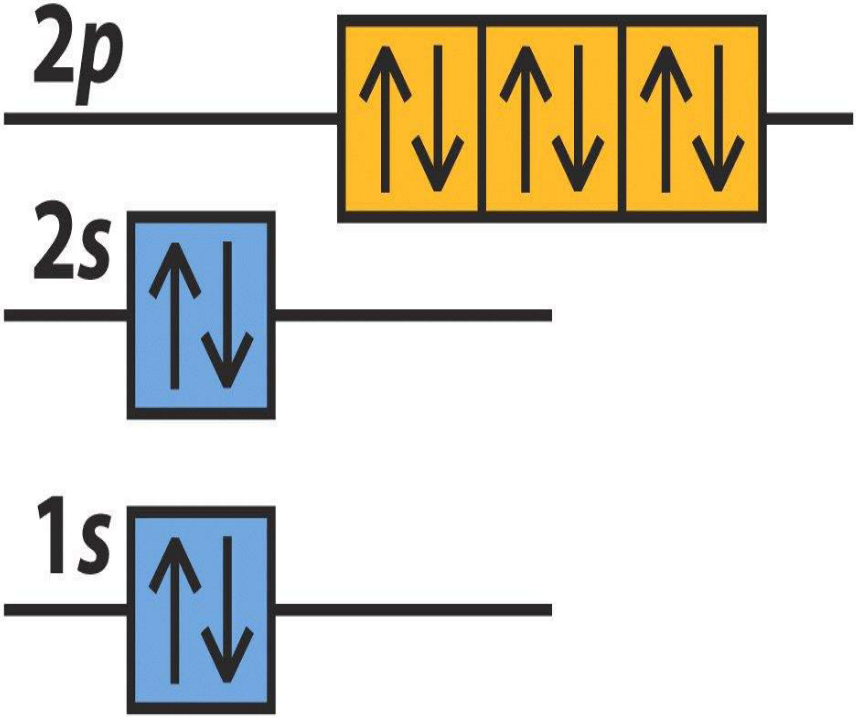
2s 2s 2s 2s

1s 1s 1s 1s

B	**C**	**N**	**O**
5	6	7	8

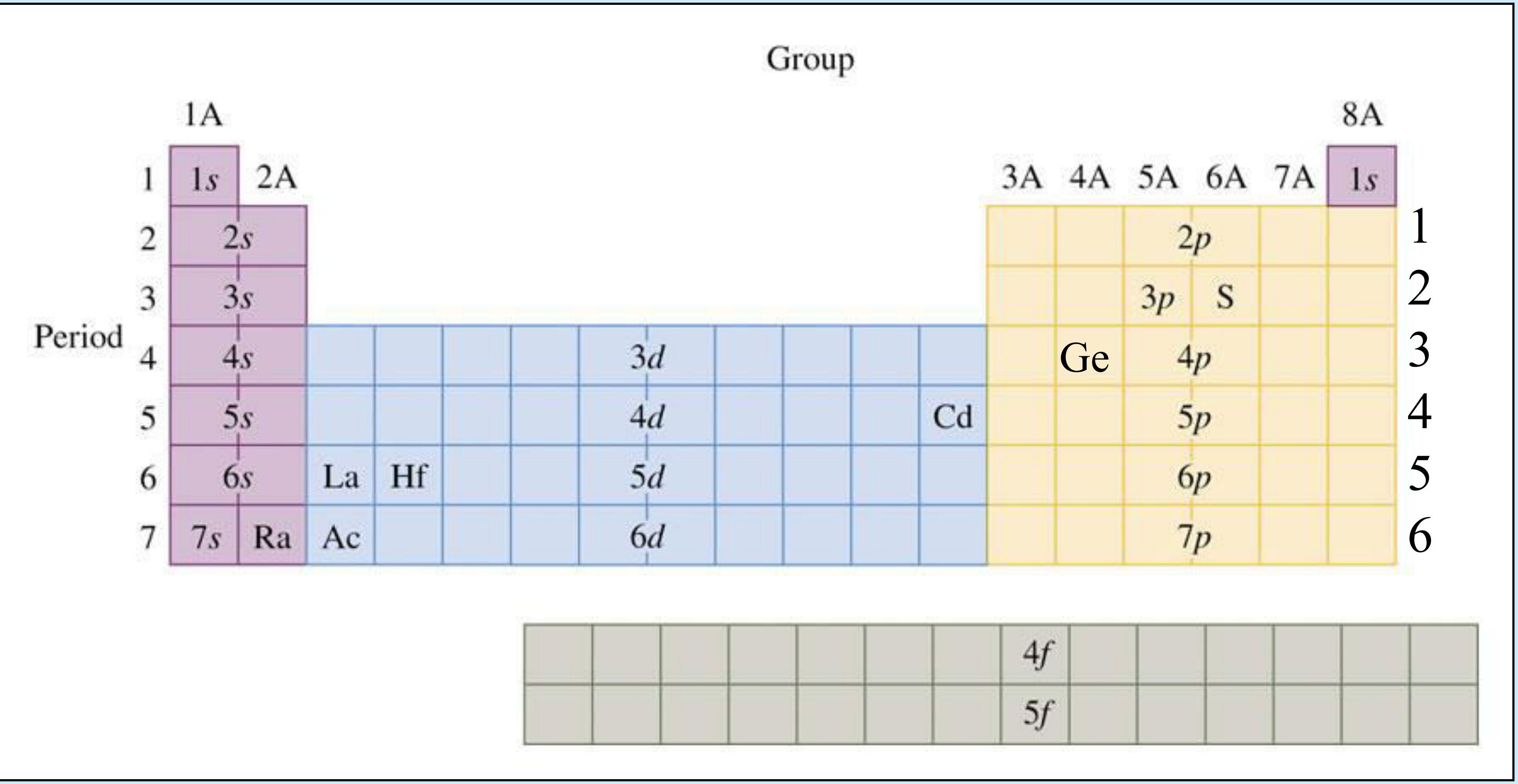


9 F $1s^2 2s^2 2p^5$, $[He]2s^2 2p^5$



10 Ne $1s^2 2s^2 2p^6$, $[\mathrm{He}]2s^2 2p^6$

2. Or you can use the periodic chart .

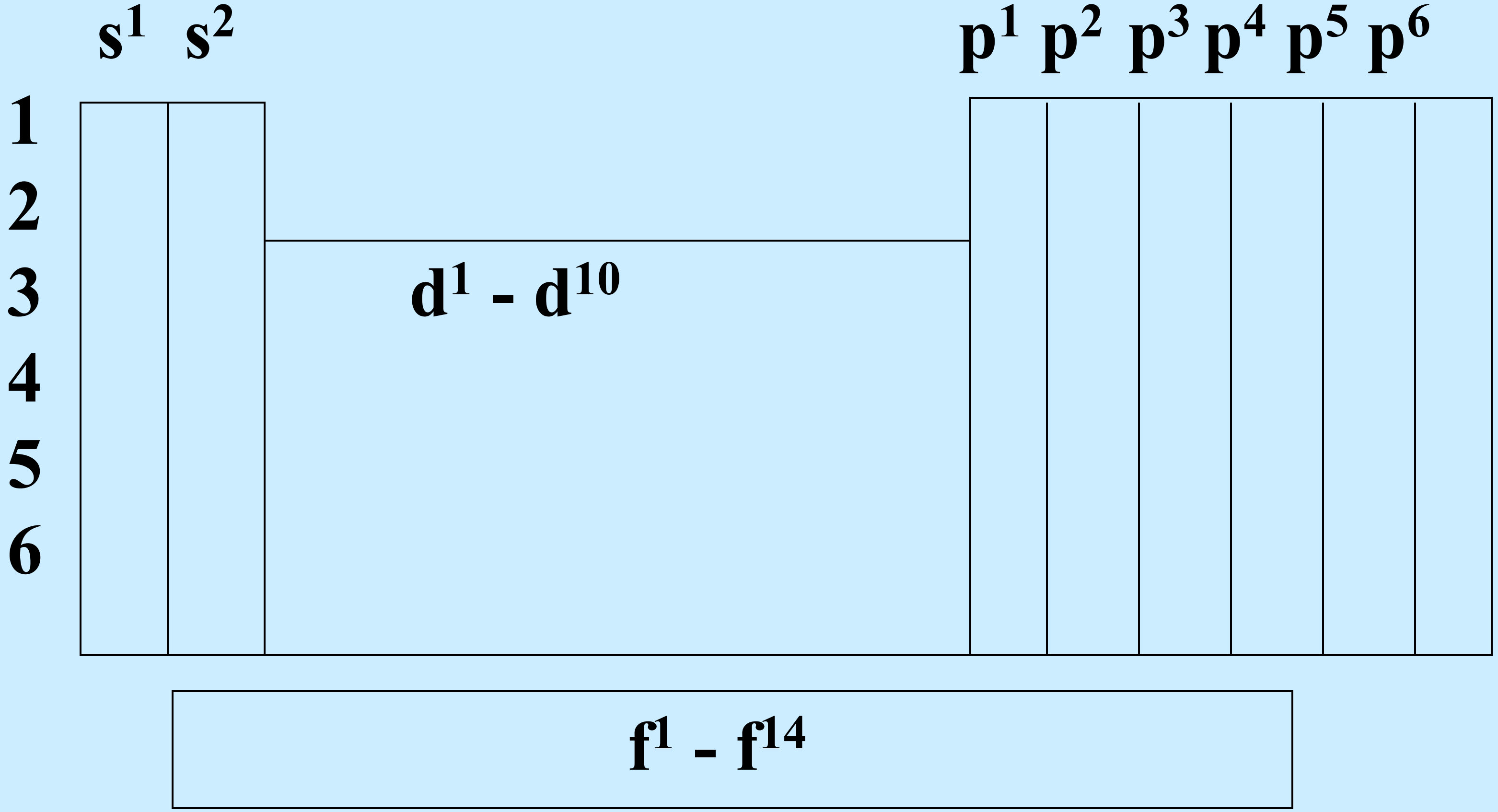


Ge = $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^2$

or $[Ar]\ 4s^2 3d^{10} 4p^2$

or $[Ar] 3d^{10}\ 4s^2 4p^2$

Sublevel Blocks



s^1 s^2

p^1 p^2 p^3 p^4 p^5 p^6

1
2
3
4
5
6

d^1 - d^{10}

f^1 - f^{14}

Hund's rule tells us that the electrons will fill the p orbitals by placing electrons in each orbital singly and with same spin until half-filled. Then the electrons will pair to finish the p orbitals.

	1s	2s	2p	Configuration	
$_{3}$Li	↑↓	↑	_ _ _	$1s^2\ 2s^1$	Paramagnetic
$_{4}$Be	↑↓	↑↓	_ _ _	$1s^2\ 2s^2$	Paramagnetic
$_{5}$B	↑↓	↑↓	↑ _ _	$1s^2\ 2s^2\ 2p^1$	Paramagnetic
$_{6}$C	↑↓	↑↓	↑ ↑ _	$1s^2\ 2s^2\ 2p^2$	Paramagnetic
$_{7}$N	↑↓	↑↓	↑ ↑ ↑	$1s^2\ 2s^2\ 2p^3$	Paramagnetic
$_{8}$O	↑↓	↑↓	↑↓ ↑ ↑	$1s^2\ 2s^2\ 2p^4$	Paramagnetic
$_{9}$F	↑↓	↑↓	↑↓ ↑↓ ↑	$1s^2\ 2s^2\ 2p^5$	Paramagnetic
$_{10}$Ne	↑↓	↑↓	↑↓ ↑↓ ↑↓	$1s^2\ 2s^2\ 2p^6$	Diamagnetic

- 3rd row elements

		3s	3p			Configuration
$_{11}\mathrm{Na}$	[Ne]	↑	_	_	_	$[\mathrm{Ne}]3s^1$
$_{12}\mathrm{Mg}$	[Ne]	↑↓	_	_	_	$[\mathrm{Ne}]3s^2$
$_{13}\mathrm{Al}$	[Ne]	↑↓	↑	_	_	$[\mathrm{Ne}]3s^2\ 3p^1$
$_{14}\mathrm{Si}$	[Ne]	↑↓	↑	↑	_	$[\mathrm{Ne}]3s^2\ 3p^2$
$_{15}\mathrm{P}$	[Ne]	↑↓	↑	↑	↑	$[\mathrm{Ne}]3s^2\ 3p^3$
$_{16}\mathrm{S}$	[Ne]	↑↓	↑↓	↑	↑	$[\mathrm{Ne}]3s^2\ 3p^4$
$_{17}\mathrm{Cl}$	[Ne]	↑↓	↑↓	↑↓	↑	$[\mathrm{Ne}]3s^2\ 3p^5$
$_{18}\mathrm{Ar}$	[Ne]	↑↓	↑↓	↑↓	↑↓	$[\mathrm{Ne}]3s^2\ 3p^6$

Fourth row

	3d	4s	4p	Configuration
$_{19}$K [Ar]	_ _ _ _ _	↑	_ _ _	$[Ar]4s^1$
$_{20}$Ca [Ar]	_ _ _ _ _	↑↓	_ _ _	$[Ar]4s^2$
$_{21}$Sc [Ar]	↑ _ _ _ _	↑↓	_ _ _	$[Ar]4s^2\ 3d^1$
$_{22}$Ti [Ar]	↑ ↑ _ _ _	↑↓	_ _ _	$[Ar]4s^2\ 3d^2$
$_{23}$V [Ar]	↑ ↑ ↑ _ _	↑↓	_ _ _	$[Ar]4s^2\ 3d^3$
$_{24}$Cr [Ar]	↑ ↑ ↑ ↑ ↑	↑	_ _ _	$[Ar]4s^1\ 3d^5$

There is an extra measure of stability associated with half-filled and completely filled orbitals.

Fourth row

	3d					4s	4p			Configuration
$_{25}$Mn [Ar]	↑	↑	↑	↑	↑	↑↓				[Ar]$4s^2\,3d^5$
$_{26}$Fe [Ar]	↑↓	↑	↑	↑	↑	↑↓				[Ar]$4s^2\,3d^6$
$_{27}$Co [Ar]	↑↓	↑↓	↑	↑	↑	↑↓				[Ar]$4s^2\,3d^7$
$_{28}$Ni [Ar]	↑↓	↑↓	↑↓	↑	↑	↑↓				[Ar]$4s^2\,3d^8$
$_{29}$Cu [Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑				[Ar]$4s^1\,3d^{10}$

Another exception like Cr!

Fourth row

	3d	4s	4p	Configuration
$_{25}$Mn [Ar]	↑ ↑ ↑ ↑ ↑	↑↓	_ _ _	$[Ar]4s^2\ 3d^5$
$_{26}$Fe [Ar]	↑↓ ↑ ↑ ↑ ↑	↑↓	_ _ _	$[Ar]4s^2\ 3d^6$
$_{27}$Co [Ar]	↑↓ ↑↓ ↑ ↑ ↑	↑↓	_ _ _	$[Ar]4s^2\ 3d^7$
$_{28}$Ni [Ar]	↑↓ ↑↓ ↑↓ ↑ ↑	↑↓	_ _ _	$[Ar]4s^2\ 3d^8$
$_{29}$Cu [Ar]	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑	_ _ _	$[Ar]4s^1\ 3d^{10}$
$_{30}$Zn [Ar]	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓	_ _ _	$[Ar]4s^2\ 3d^{10}$

Fourth row

	3d	4s	4p	Configuration
$_{31}$Ga [Ar]	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓	↑ _ _	$[Ar]4s^2\ 3d^{10}\ 4p^1$
$_{32}$Ge [Ar]	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓	↑ ↑ _	$[Ar]4s^2\ 3d^{10}\ 4p^2$
$_{33}$As [Ar]	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓	↑ ↑ ↑	$[Ar]4s^2\ 3d^{10}\ 4p^3$
$_{34}$Se [Ar]	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓	↑↓ ↑ ↑	$[Ar]4s^2\ 3d^{10}\ 4p^4$
$_{35}$Br [Ar]	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓	↑↓ ↑↓ ↑	$[Ar]4s^2\ 3d^{10}\ 4p^5$
$_{36}$Kr [Ar]	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓	↑↓ ↑↓ ↑↓	$[Ar]4s^2\ 3d^{10}\ 4p^6$

Specific quantum numbers for each electron

	$\mathbf{n}$	ℓ	$\mathbf{m}_\ell$	$\mathbf{m}_s$
1st e^-	1	0	0	+1/2

Specific quantum numbers for each electron

	n	ℓ	m_ℓ	m_s	
1st e^-	1	0	0	+1/2	1 s electrons
2nd e^-	1	0	0	−1/2	
3rd e^-	2	0	0	+1/2	2 s electrons
4th e^-	2	0	0	−1/2	
5th e^-	2	1	-1	+1/2	2 p electrons
6th e^-	2	1	0	+1/2	
7th e^-	2	1	+1	+1/2	
8th e^-	2	1	−1	−1/2	
9th e^-	2	1	0	−1/2	
10th e^-	2	1	+1	−1/2	
11th e^-	3	0	0	+1/2	3 s electron

Chemical properties → Valence electrons

	1s	2s	2p			Configuration
$_3$Li	↑↓	↑				$1s^2\ 2s^1$
$_4$Be	↑↓	↑↓				$1s^2\ 2s^2$
$_5$B	↑↓	↑↓	↑			$1s^2\ 2s^2\ 2p^1$
$_6$C	↑↓	↑↓	↑	↑		$1s^2\ 2s^2\ 2p^2$
$_7$N	↑↓	↑↓	↑	↑	↑	$1s^2\ 2s^2\ 2p^3$
$_8$O	↑↓	↑↓	↑↓	↑	↑	$1s^2\ 2s^2\ 2p^4$