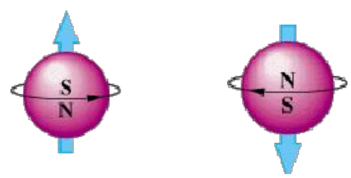
ELECTRONIC STRUCTURE OF ATOMS

Electron Spin

The electron:

- spins around its own axis
- acts as an tiny magnet (any moving electrical charge creates a magnetic field around itself)
- can spin in either of 2 directions:



- **An orbital can hold no more than two electrons with the condition that the two electrons spin in opposite directions.**

Abbreviations: $\boxed{\uparrow\downarrow}$ OR $\underline{\uparrow\downarrow}$ OR $\uparrow\downarrow$

- Reason: Two electrons spinning in the same direction would repel one another since the magnetic fields they create would repel.

- To distinguish between 2 electrons found on the same orbital, another quantum number must be introduced:

$$\mathbf{m_s = \text{spin quantum number}}$$

- There are 2 allowed values for $\mathbf{m_s}$: $\mathbf{+\frac{1}{2}}$ **and** $\mathbf{-\frac{1}{2}}$

$$m_s = +\frac{1}{2} \qquad m_s = -\frac{1}{2}$$

Recall:

- Each orbital can be identified by 3 quantum numbers:

	n	**l**	**m_l**
	principal quantum number	secondary quantum number	magnetic quantum number
Indicates →	Energy level	shape of orbital	orientation of orbital

CONCLUSION:

- Each electron can be identified by 4 quantum numbers:

	n	**l**	**m_l**	**m_s**
	principal quantum number	secondary quantum number	magnetic quantum number	spin quantum number
Indicates →	Energy level	shape of orbital	orientation of orbital	direction of spin

- Since an orbital can hold no more than 2 electrons (only if they have opposite spins)

  It follows: **NO TWO ELECTRONS IN AN ATOM CAN HAVE THE SAME 4 QUANTUM NUMBERS**
  (Pauli's exclusion principle)

- It follows that the maximum number of electrons in a particular sublevel (subshell) is limited.

Secondary quantum no.	Subshell designation	Number of orbitals	Maximum number of electrons
l = 0	s	1	2
l = 1	p	3	6
l =2	d	5	10
l =3	f	7	14

- The maximum number of sublevels (subshells), orbitals and electrons in any energy level can now easily be predicted:

Energy level	Number of sublevels	Sublevel Designation	Number of orbitals	Maximum number of electrons
n=1	1	1s	1	2
n=2	2	2s, 2p	4	8
n=3	3	3s, 3p, 3d	9	18
n=4	4	4s, 4p, 4d, 4f	16	32
n=5	5	5s, 5p, 5d, 5f, 5g	25	50
For any n	**n**		**n^2**	**$2n^2$**

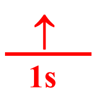
- **Every atom has an infinite number of possible electron configurations**.

Ground State
The electron configuration associated with the lowest energy level of an atom

Excited States
The electron configurations associated with energy levels higher than the lowest

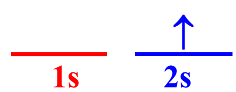
Example:

Ground State electron configuration of H atom

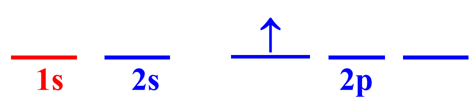


or **$1s^1$**

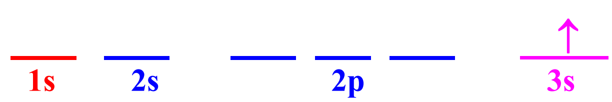
Excited State electron configurations of H of H atom



or **$2s^1$**



or **$2p^1$**



or **$3s^1$**

- **The chemical properties of an atom are related to the electron configuration of its ground state**

Ground State Electron Configurations of Elements

- Follows the **"AUFBAU PRINCIPLE"** (Aufbau = building up)

- **In an atom in its ground state, the electrons will be found in the lowest energy levels (respectively sublevels) available.**

Period 1 Elements:

Z	Element	Orbital Diagram	Electron Configuration
1	H	$\underset{1s}{\underline{\uparrow}}$	$1s^1$
2	He	$\underset{1s}{\underline{\uparrow\downarrow}}$	$1s^2$
Note: The orbital is complete The 2s subshell (sublevel) is complete The 1st energy level is complete			

Period 2 Elements:

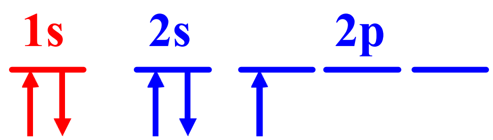
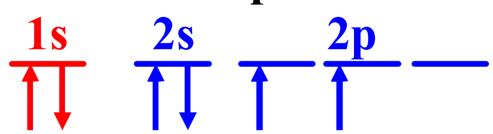
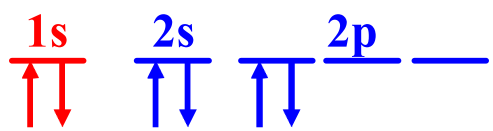
Z	Element	Orbital Diagram	Electron Configuration
3	Li	$\underset{1s}{\underline{\uparrow\downarrow}}$ $\underset{2s}{\underline{\uparrow}}$	$1s^2\,2s^1$
4	Be	$\underset{1s}{\underline{\uparrow\downarrow}}$ $\underset{2s}{\underline{\uparrow\downarrow}}$	$1s^2\,2s^2$

core electrons

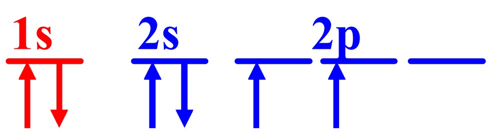
valence electrons

- **Common abbreviated electron configuration of Be that uses Noble Gas symbol:**

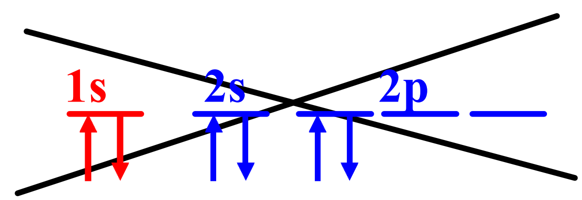
[He] $\underset{2s}{\underline{\uparrow\downarrow}}$ and **[He] $2s^2$**

Z	Element	Orbital Diagram	Electron Configuration
5	**B**		**$1s^2$ $2s^2$ $2p^1$ or [He] $2s^2 2p^1$**
6	**C**	**There are 2 possibilities:**  	**$1s^2$ $2s^2$ $2p^2$ or [He] $2s^2 2p^2$**

- The correct orbital diagram(electron configuration) is determined by **"HUND'S RULE"**
- **Electrons entering a subshell containing more than one orbital will be spread out over the available equal-energy orbitals with their spins in the same direction**
- (Rule of "unfriendly electrons")



CORRECT



INCORRECT

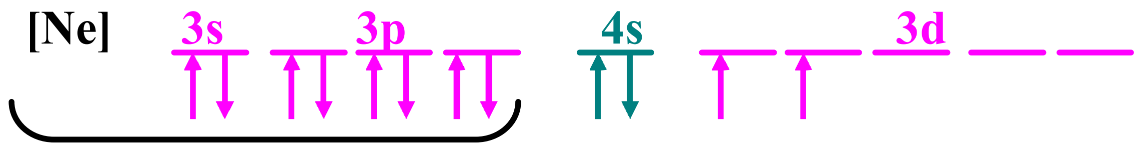
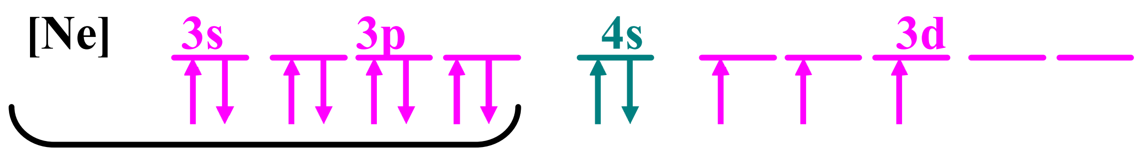
Z	Orbital Diagram		Electron Configuration
7	N	1s: $\uparrow\downarrow$ 2s: $\uparrow\downarrow$ 2p: $\uparrow$ $\uparrow$ $\uparrow$ 5 outermost shell electrons (3 unpaired)	$1s^2\ 2s^2\ 2p^3$ or [He] $2s^2\ 2p^3$
8	O	1s: $\uparrow\downarrow$ 2s: $\uparrow\downarrow$ 2p: $\uparrow\downarrow$ $\uparrow$ $\uparrow$ 6 outermost shell electrons (2 unpaired)	$1s^2\ 2s^2\ 2p^4$ or [He] $2s^2\ 2p^4$
9	F	1s: $\uparrow\downarrow$ 2s: $\uparrow\downarrow$ 2p: $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow$ 7 outermost shell electrons (1 unpaired)	$1s^2\ 2s^2\ 2p^5$ or [He] $2s^2\ 2p^5$

Z		Orbital Diagram	Electron Configuration
10	Ne	1s: ↑↓ 2s: ↑↓ 2p: ↑↓ ↑↓ ↑↓ $\underbrace{\text{1s}}_{\text{2e's}}$ $\underbrace{\text{2s 2p}}_{\text{8 e's}}$	$1s^2$ $2s^2$ $2p^6$ or [He] $2s^2$ $2p^6$
NOTE: The 1st and the 2nd energy levels are complete (filled to capacity)			
11	Na	1s: ↑↓ 2s: ↑↓ 2p: ↑↓ ↑↓ ↑↓ 3s: ↑ 10 core electrons (2 complete inner shels) (electron configuration of Ne) 1 electron on outermost shell (3rd shell)	$1s^2$ $2s^2$ $2p^6$ $3s^1$ or [Ne] $3s^1$
12	Mg	1s: ↑↓ 2s: ↑↓ 2p: ↑↓ ↑↓ ↑↓ 3s: ↑↓ 10 core electrons (2 complete inner shels) (electron configuration of Ne) 2 electrons on outermost shell (3rd shell)	$1s^2$ $2s^2$ $2p^6$ $3s^2$ or [Ne] $3s^2$

Z		Orbital Diagram	Electron Configuration
13	Al	1s ↑↓ 2s ↑↓ 2p ↑↓ ↑↓ ↑↓ 3s ↑↓ 3p ↑ __ __ 10 core electrons (2 complete inner shels) 3 electrons on outermost shell (3rd shell)	$1s^2\ 2s^2\ 2p^6\ 3s^2$ or [Ne] $3s^2\ 3p^1$
14	Si	[Ne] 3s ↑↓ 3p ↑ ↑ __ Recall "Hund's Rule" (Rule of unfriendly electrons)	[Ne] $3s^2\ 3p^2$ 2 complete energy levels 4 electrons on outermost shell
15	P	[Ne] 3s ↑↓ 3p ↑ ↑ ↑ 2 complete energy levels (10 electrons) 5 electrons on outermost shell (3 unpaired electrons)	[Ne] $3s^2\ 3p^3$

Z		Orbital Diagram	Electron Configuration
16	**S**	**[Ne]** 3s ↑↓ 3p ↑↓ ↑ ↑ **2 complete energy levels (10 electrons)** 6 electrons on outermost shell (2 unpaired electrons)	**[Ne]** $3s^2\ 3p^4$
17	**Cl**	**[Ne]** 3s ↑↓ 3p ↑↓ ↑↓ ↑ **2 complete energy levels (10 electrons)** 7 electrons on outermost shell (1 unpaired electron)	**[Ne]** $3s^2\ 3p^5$
18	**Ar**	**[Ne]** 3s ↑↓ 3p ↑↓ ↑↓ ↑↓ **2 complete energy levels (10 electrons)** 8 electrons on outermost shell (no unpaired electrons)	**[Ne]** $3s^2\ 3p^6$

Z	Element	Orbital Diagram	Electron Configuration
19	K	$\underbrace{[Ne]\ \overset{3s}{\uparrow\downarrow}\ \overset{3p}{\uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow}}_{\text{Electronic Configuration of Ar}}\ \underbrace{\overset{4s}{\uparrow}}_{\text{1 outermost shell electron}}$	$\underbrace{[Ne]\ 3s^2 3p^6}_{Ar}\ 4s^1$ or $[Ar]\ 4s^1$
20	Ca	$\underbrace{[Ne]\ \overset{3s}{\uparrow\downarrow}\ \overset{3p}{\uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow}}_{\text{Electronic Configuration of Ar}}\ \underbrace{\overset{4s}{\uparrow\downarrow}}_{\text{2 outermost shell electrons}}$	$\underbrace{[Ne]\ 3s^2 3p^6}_{Ar}\ 4s^2$ or $[Ar]\ 4s^2$
21	Sc	$\underbrace{[Ne]\ \overset{3s}{\uparrow\downarrow}\ \overset{3p}{\uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow}}_{\text{Electronic Configuration of Ar}}\ \underbrace{\overset{4s}{\uparrow\downarrow}}_{\text{2 outermost shell electrons}}\ \overset{3d}{\uparrow\ \_\ \_\ \_\ \_}$ Recall: 3d sublevel is higher in energy than 4s	$[Ar]\ 4s^2\ 3d^1$

Z	Element	Orbital Diagram	Electron Configuration
22	**Ti**	 **Electronic Configuration of Ar** **2 outermost shell electrons** **Recall: Hund's Rule (Rule of "unfriendly electrons)**	**[Ar] $4s^2$ $3d^2$**
23	**V**	 **Electronic Configuration of Ar** **2 outermost shell electrons** **Recall: Hund's Rule (Rule of "unfriendly electrons)**	**[Ar] $4s^2$ $3d^3$**

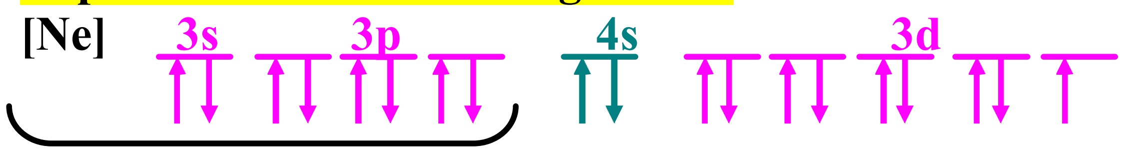
Exceptions to the Building-Up Principle

Cr (Z = 24)	**Expected Electronic Configuration:** **[Ne]** 3s: ↑↓ 3p: ↑↓ ↑↓ ↑↓ 4s: ↑↓ 3d: ↑ ↑ ↑ ↑ _ **Electronic Configuration of Ar** — **2 outermost shell electrons**	**[Ar] $4s^2\ 3d^4$**
	Actual Electronic Configuration: **[Ne]** 3s: ↑↓ 3p: ↑↓ ↑↓ ↑↓ 4s: ↑ 3d: ↑ ↑ ↑ ↑ ↑ **Electronic Configuration of Ar** — **1 outermost shell electron**	**[Ar] $4s^1\ 3d^5$**
	Reason: The actual electronic configuration is lower in energy and thus more stable because of the extra stability associated with a large half-filled 3d subshell: 3d: ↑ ↑ ↑ ↑ ↑	

Cu (Z = 29)

Expected Electronic Configuration:

[Ne]

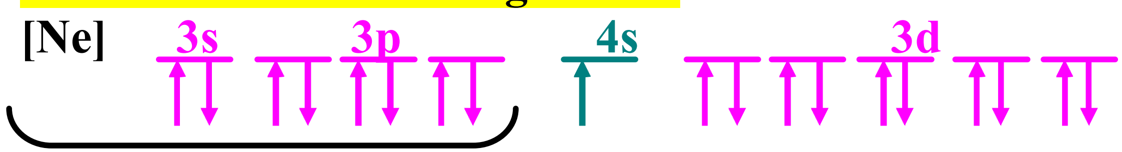


[Ar] $4s^2$ $3d^9$

Electronic Configuration of Ar **2 outermost shell electrons**

Actual Electronic Configuration:

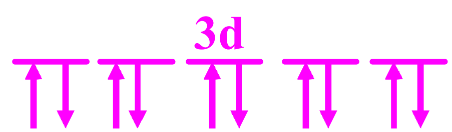
[Ne]



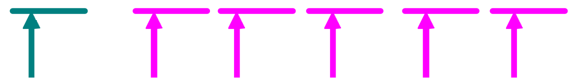
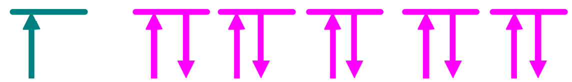
[Ar] $4s^1$ $3d^{10}$

Electronic Configuration of Ar **1 outermost shell electron**

Reason: The actual electronic configuration is lower in energy and thus more stable because of the extra stability associated with a large filled 3d subshell:



Other exceptions:

Mo (Z = 42)	[Kr] 5s 4d  extra-stability associated with a half-filled subshell	[Kr] $5s^1$ $4d^5$
Ag (Z = 47)	[Kr] 5s 4d  extra-stability associated with a filled subshell	[Kr] $5s^1$ $4d^{10}$

- For atoms with a large atomic number (many electrons), irregular electronic configurations are quite common.
- Reason: As the number of energy levels increases, the outer subshells are relatively close to each other. The electrons can easily move to one subshell to another to adopt the configuration with the lowest energy (most stable configuration)