

ELECTRON CONFIGURATION

Electron Configuration

Electron configuration is a shorthand notation for describing the arrangement of the electrons about the nucleus.

General Format using the quantum numbers:

$n \ell e^-$

n = principle quantum number

ℓ = angular momentum quantum number

e^- = number of electrons

RULES:

1. Fill the lowest energy levels first.



1s 2s 2p 3s 3p 4s 3d 4p

2. No more than two electrons per orbital.

Electron Configuration

Examples:

H: $1s^1$

He: $1s^2$

Li: $1s^2 2s^1$

Co: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^7$

Br: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^5$

The condensed electron configuration distinguishes the core electrons from the valence electrons. **CORE electrons are tightly held to the nucleus and resemble a noble gas configuration.** **VALENCE** electrons are the outer most electrons and are involved in chemical reactions.

Examples of the condensed configuration:

Li: **[He]** $2s^1$

Co: **[Ar]** $4s^2 3d^7$

Br: **[Ar]** $4s^2 3d^{10} 4p^5$

A few principles to consider:

Aufbau Principle: The procedure for arriving at the ground-state electron configurations of atoms and molecules in order of increasing atomic number. To proceed from one atom to the next, we add a proton and some neutrons to the nucleus and then describe the orbital into which the added electron goes.

Hund's Rule: Whenever orbitals of equal energy (degenerate) are available, electrons occupy these orbitals singly before pairing begins.

Core vs. Valence electrons: inner vs. outermost electrons (latter contained within outermost shell)

5

Electron Configuration from the Periodic Table

	1A																	8A
1		2A																
2																		
3																		Ne
4																		
5																		
6																		
7																		

Si = [Ne]3s²3p²
 Si has 4 valence electrons

Electron Configuration from the Periodic Table

	1A																	8A
1		2A																
2																		
3																		
4																		
5																		
6																		
7																		



P has 5 valence electrons

Electron Configuration from the Periodic Table

	1A																8A
1		2A															
2																	
3																	
4																	
5																	
6																	
7																	

Cl = [Ne]3s²3p⁵
 Cl has 7 valence electrons

LECTURE QUIZ #15A on Electron Configuration

- 1) Write the full electron configuration for Cl/Ar/Ca.
- 2) Write the shorthand configuration for Cl/Ar/Ca and circle the valence electrons?

Sublevel Splitting in Multielectron Atoms

- the sublevels in each principal energy level of Hydrogen all have the same energy – we call orbitals with the same energy **degenerate**
 - or other single electron systems
- for multielectron atoms, the energies of the sublevels are split
 - caused by electron-electron repulsion
- the lower the value of the l quantum number, the less energy the sublevel has
 - $s (l = 0) < p (l = 1) < d (l = 2) < f (l = 3)$

APPLICATION OF QUANTUM CHEMISTRY – The multi-electron atom

subshells

shielded

effective nuclear charge, Z_{eff} ,

penetrate

order : $s < p < d < f$.

Many-Electron Atoms

We need to examine the balance of attractions and repulsions in the atom to explain why **subshells** of a given shell have different energies.

Each electron in a many-electron atom is repelled by the other electrons present, as well as being attracted by the nucleus. This results in that electron being *less* tightly bound to the nucleus than it would be if those other electrons were absent.

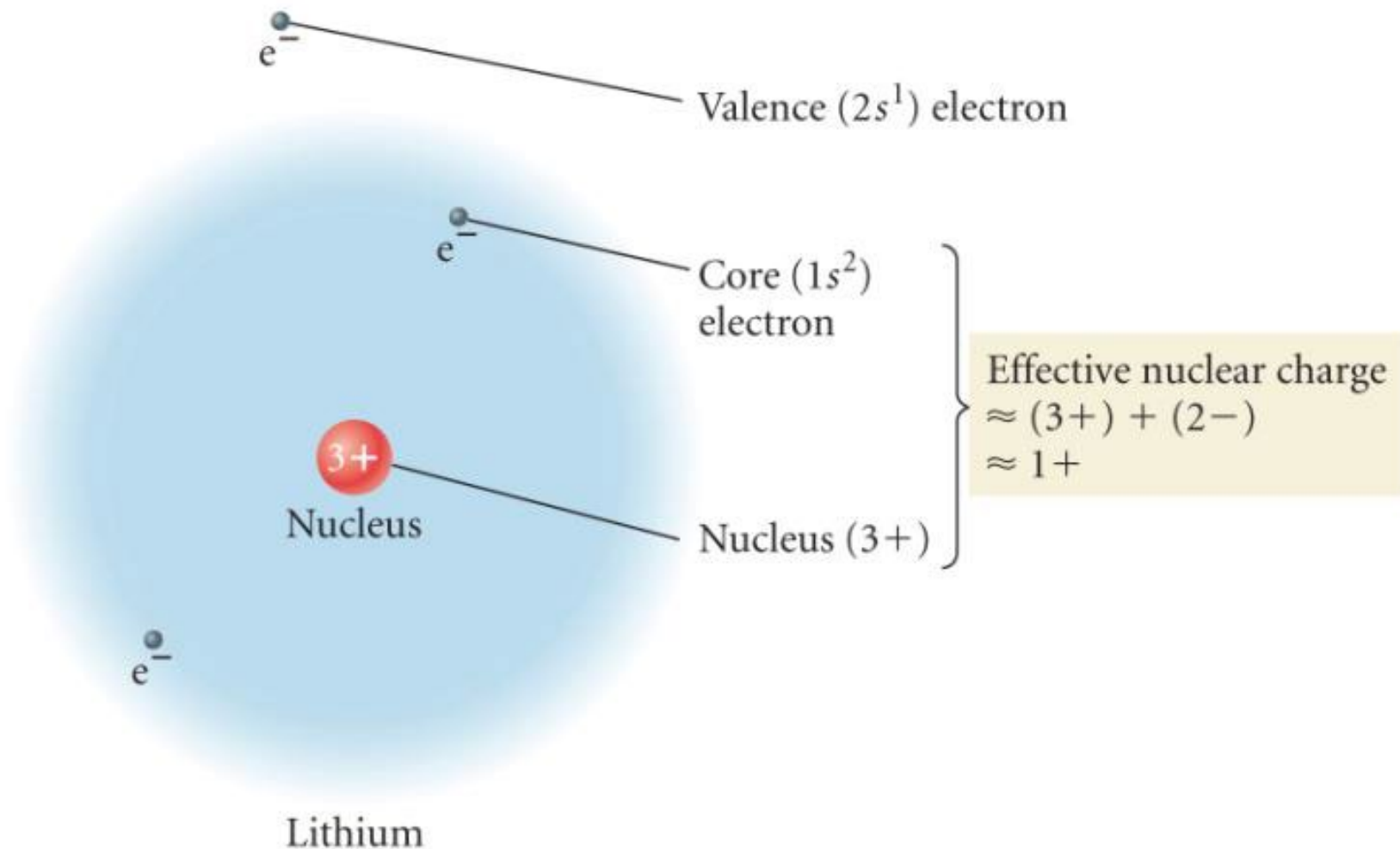
We say that each electron is **shielded** from the full attraction of the nucleus by the other electrons in the atom.

The shielding effectively reduces the pull of the nucleus on an electron. The effective nuclear charge, Z_{eff} experienced by the electron is always less than the actual nuclear charge, Z , because the electron-electron repulsions work against the pull of the nucleus.

Note that the other electrons do not “block” the influence of the nucleus; they simply provide additional repulsive Coulombic interactions that partly counteract the pull of the nucleus.

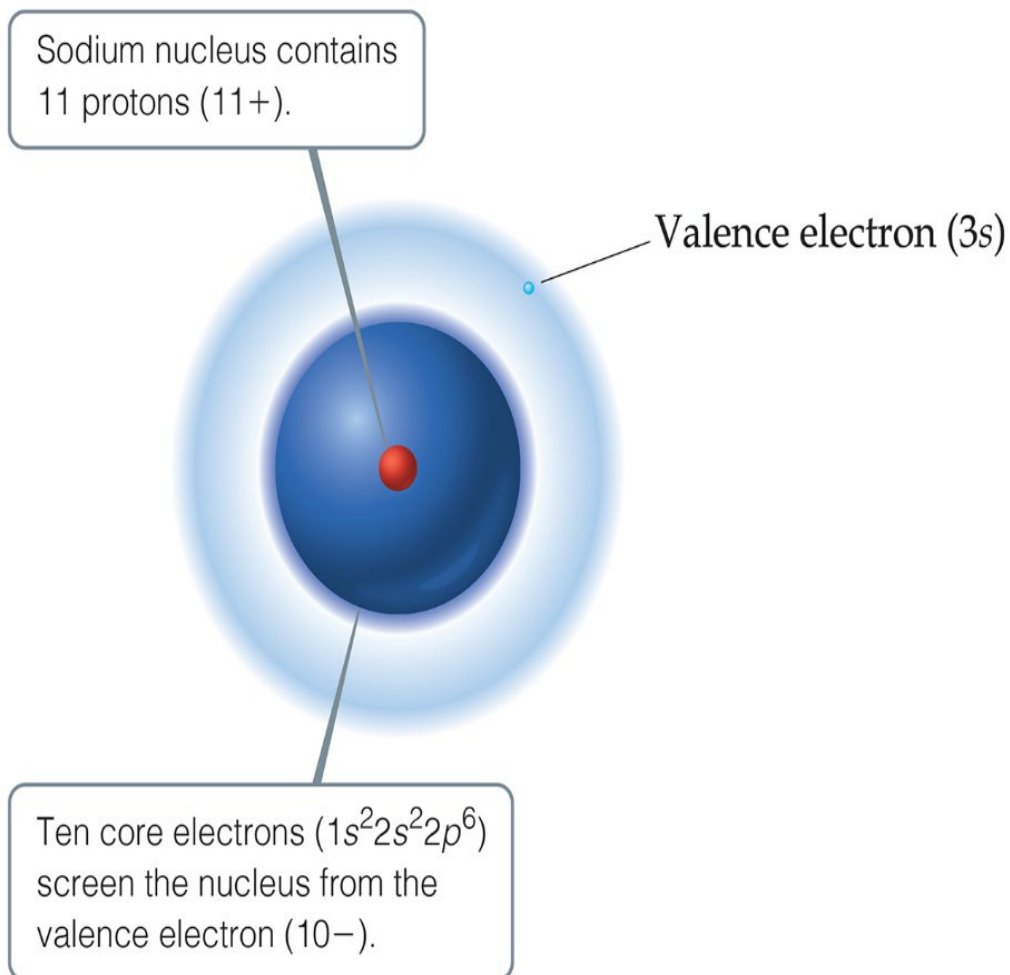
Screening & Effective Nuclear Charge₂

Screening and Effective Nuclear Charge



Effective Nuclear Charge

- Many properties depend on attractions between valence electrons and the nucleus.
- Electrons are both attracted to the nucleus and repelled by other electrons.
- The forces an electron experiences depend on both factors.



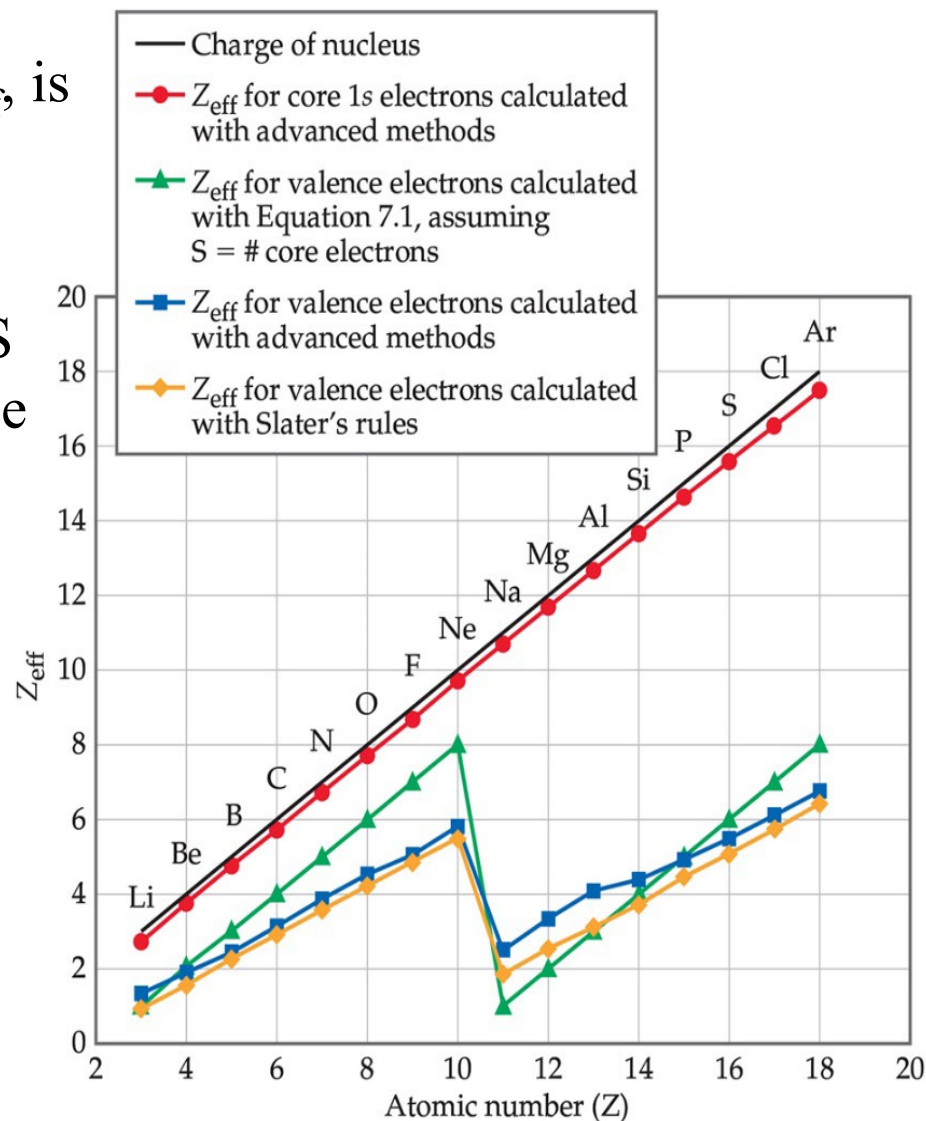
Effective Nuclear Charge

- The effective nuclear charge, Z_{eff} , is found this way:

$$Z_{\text{eff}} = Z - S$$

where Z is the atomic number and S is a screening constant, usually close to the number of inner electrons.

- Effective nuclear charge is a periodic property:
 - It increases across a period.
 - It increases **slightly** down a group.



Many-Electron Atoms

Finally, an s -electron of any shell can be found very close to the nucleus, so we say that it can **penetrate** through the inner shells. A p -electron penetrates much less.

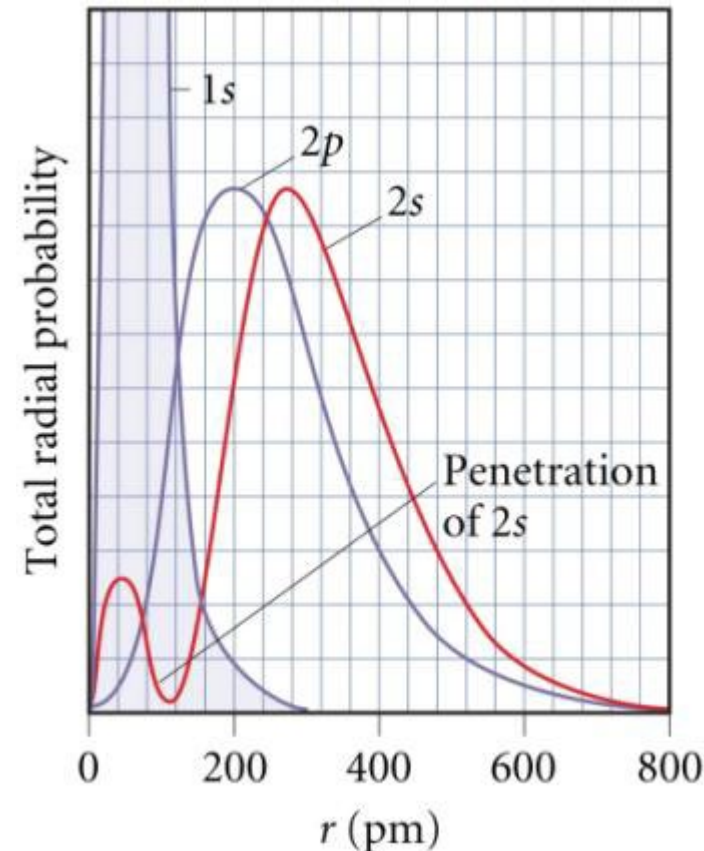
Due to the p -electron penetrating less than an s -electron through the inner shells of the atom, it is more effectively **shielded** from the nucleus and hence experiences a *smaller effective nuclear charge* than an s -electron does.

That is, an s -electron is bound more tightly than a p -electron and has a slightly lower (more negative) energy.

In a many-electron atom, because of the effects of penetration and shielding, the order of energies of orbitals in a given shell is typically $s < p < d < f$.

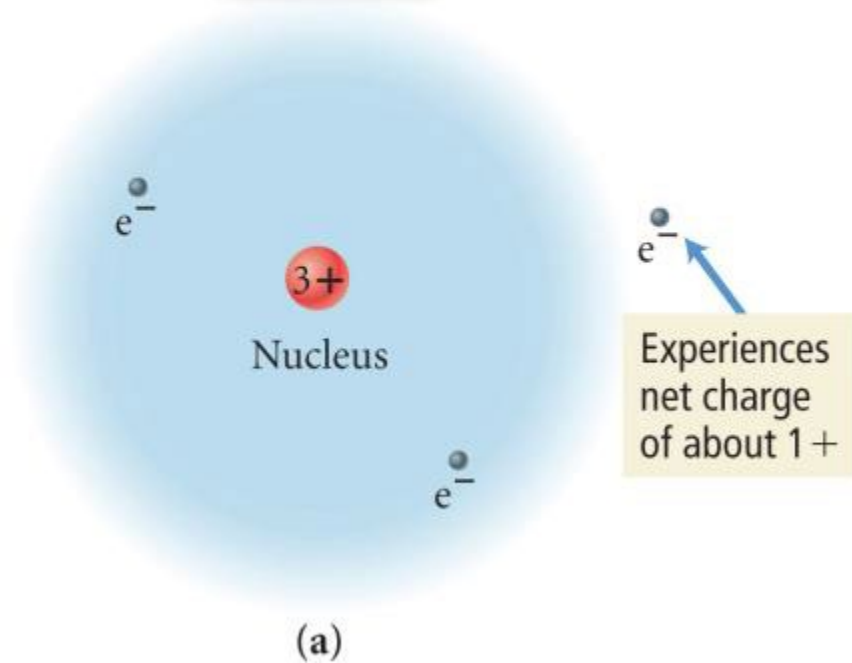
Penetrating and Shielding

- the radial distribution function shows that the $2s$ orbital penetrates more deeply into the $1s$ orbital than does the $2p$
- the weaker penetration of the $2p$ sublevel means that electrons in the $2p$ sublevel experience more repulsive force, they are more shielded from the attractive force of the nucleus
- the deeper penetration of the $2s$ electrons means electrons in the $2s$ sublevel experience a greater attractive force to the nucleus and are not shielded as effectively
- the result is that the electrons in the $2s$ sublevel are lower in energy than the electrons in the $2p$

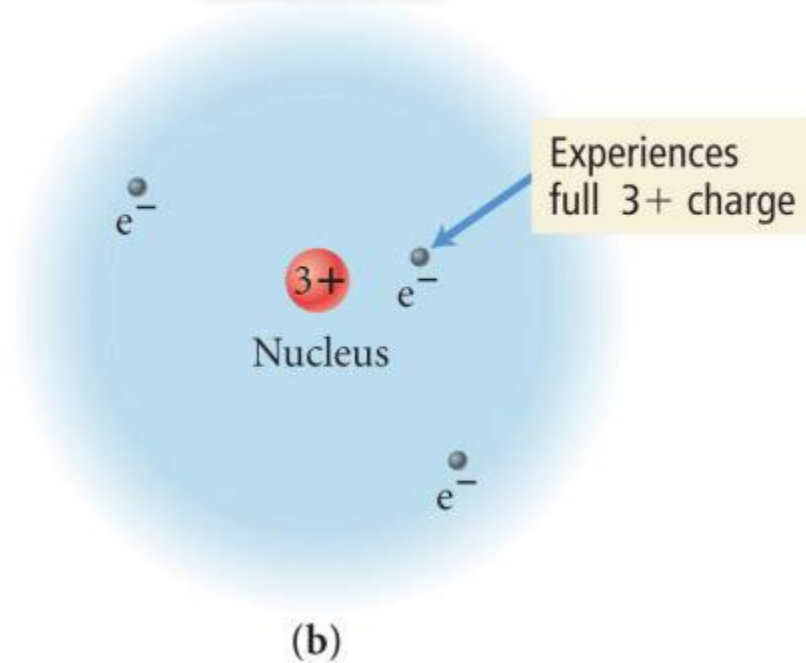


Penetration & Shielding

Shielding

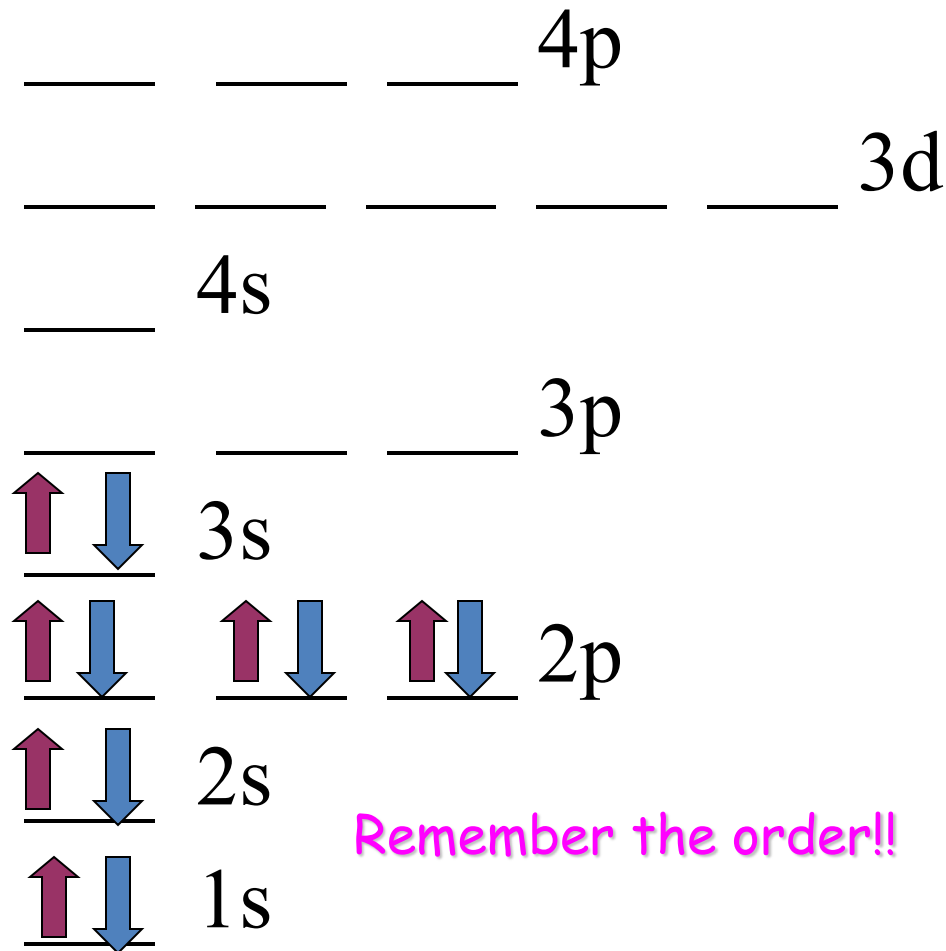


Penetration



Orbital Diagrams

Orbital diagrams are written in order of increasing energy levels starting with the lowest energy level the 1s orbital.

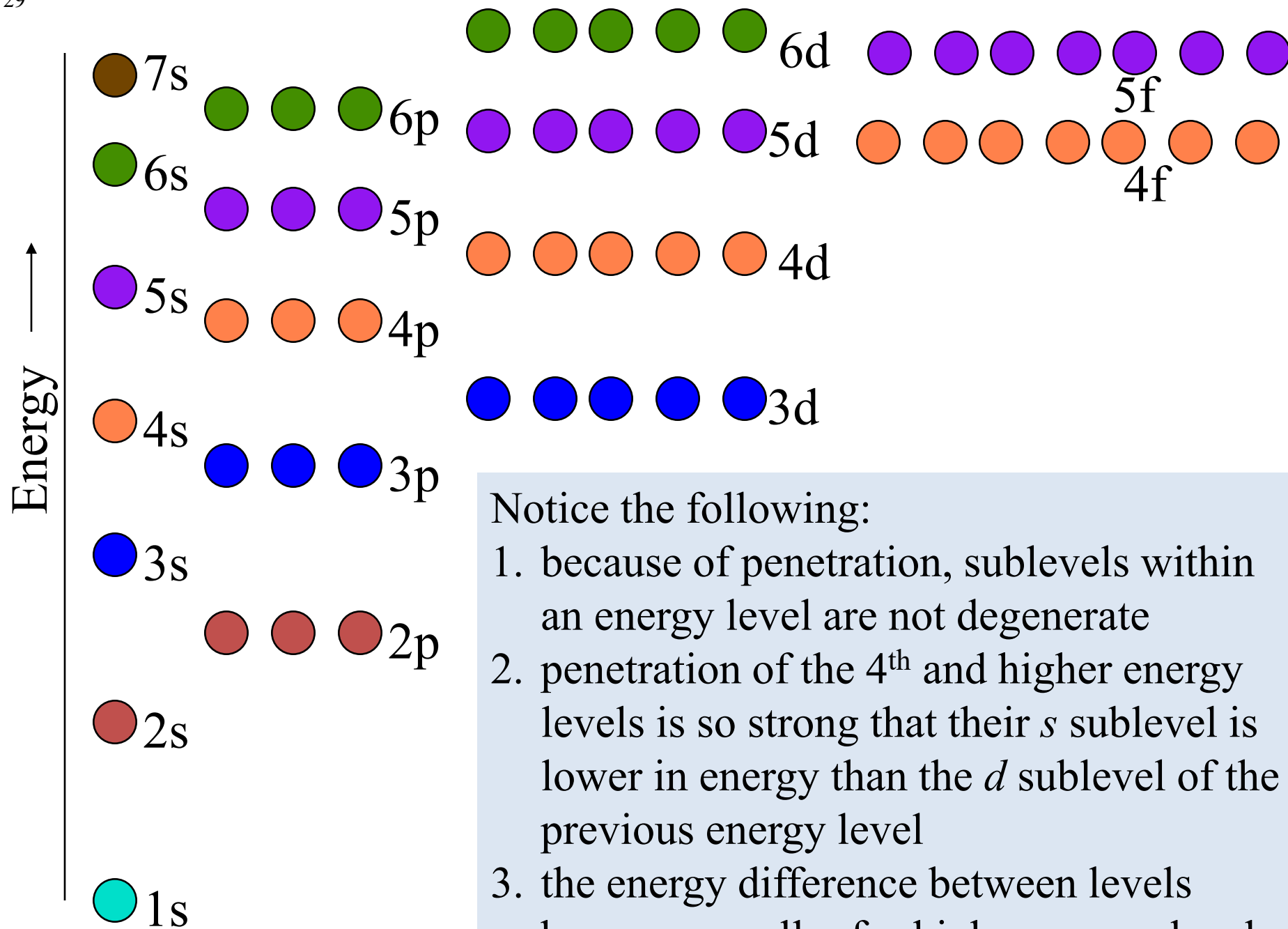


RULES:

(1) fill the lowest energy level first

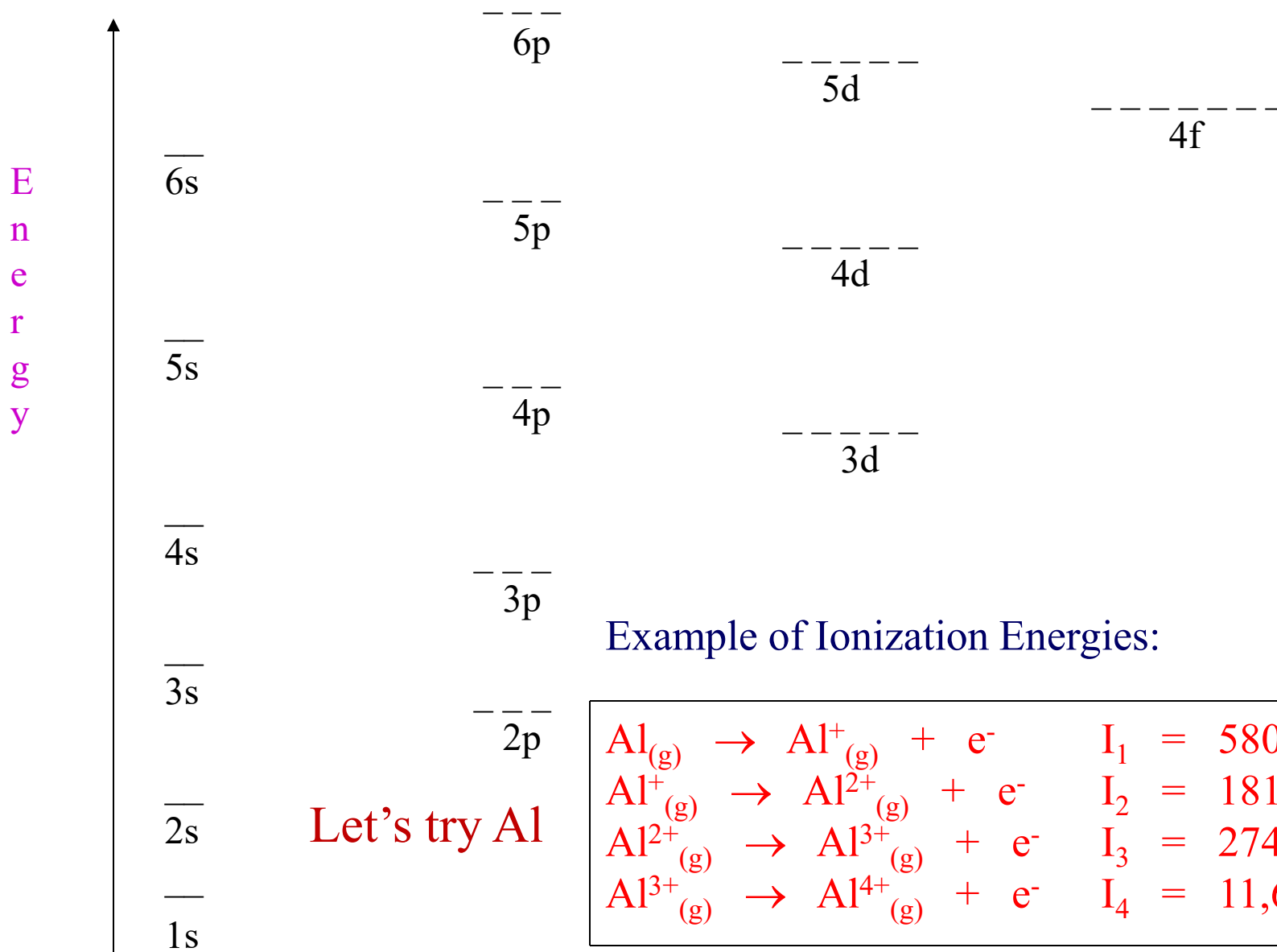
(2) fill each orbital in a subshell with one electron first before you double up.

(3) Completely fill each subshell before proceeding to the next energy level.



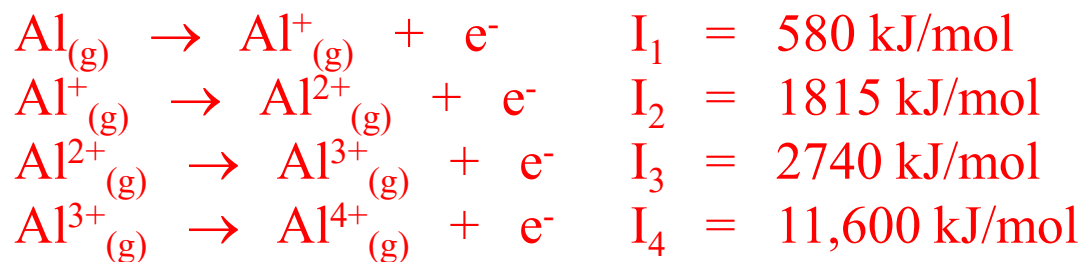
QUANTUM MECHANICS & ORBITAL DIAGRAMS

Orbital Energy Levels:



Example of Ionization Energies:

Let's try Al



Iron Configuration from the Periodic Table

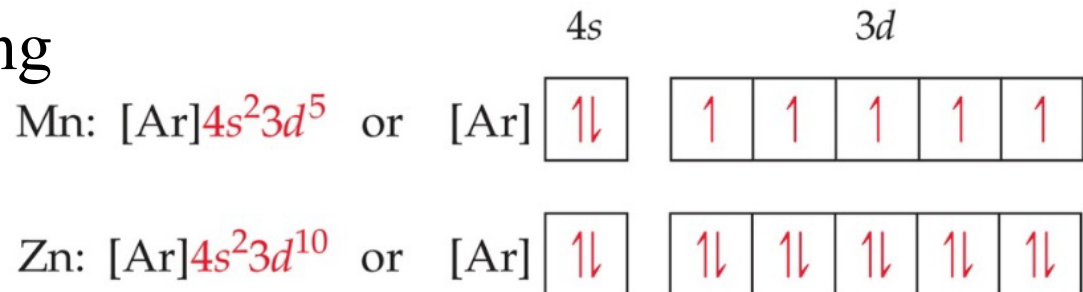
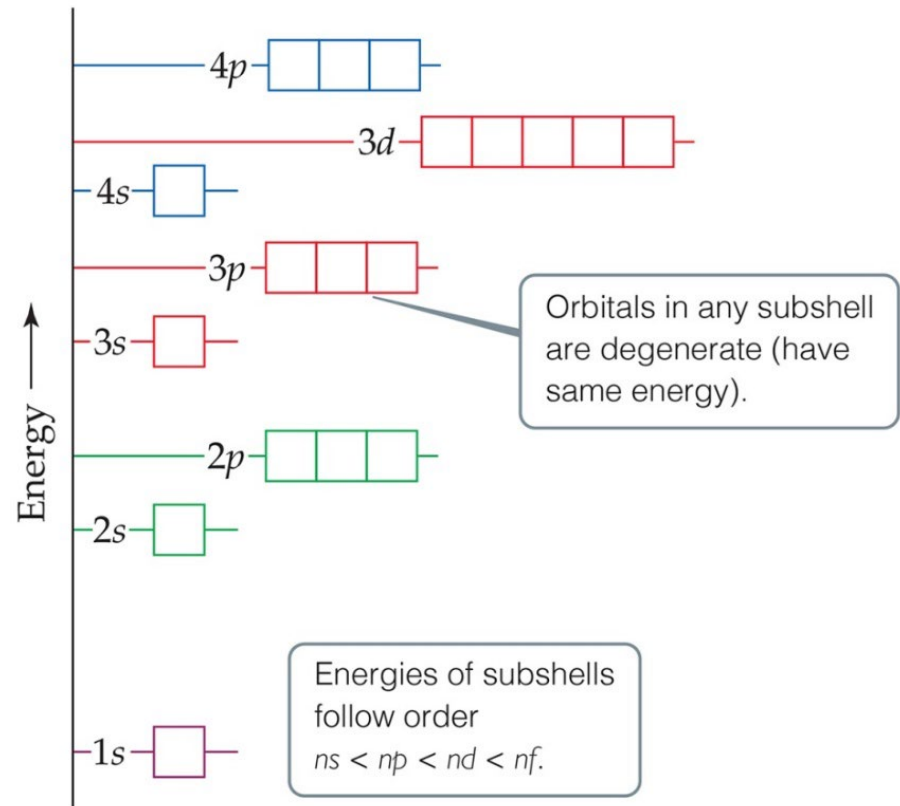
The diagram illustrates the periodic table with the following labels and features:

- Columns (Groups):** 1A, 2A, 3A, 4A, 5A, 6A, 7A, 8A.
- Rows (Periods):** 1, 2, 3, 4, 5, 6, 7.
- Orbital Filling:**
 - $4s^2$ is indicated in the 4th period, 2A group.
 - $3d^{10}$ is indicated in the 4th period, 10th column.
 - $4p^3$ is indicated in the 4th period, 15th column.
- Other Labels:** Ar (Argon) is labeled in the 3rd period, 8A group.



Transition Metals

- Argon (atomic number 18) ends period 3. Its electron configuration is $1s^2 2s^2 2p^6 3s^2 3p^6$.
- Potassium (atomic number 19) might be expected to have electrons in $3d$. **But** $4s$ fills next.
- Transition metals** follow the filling of $4s$ by filling $3d$ in the 4th period. Mn: [



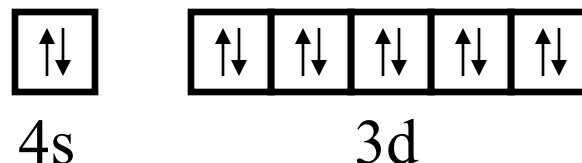
Transition Elements

- for the *d* block metals, the principal energy level is one less than valence shell
 - one less than the Period number
 - sometimes *s* electron “promoted” to *d* sublevel

Zn

$Z = 30$, Period 4, Group 2B

$[\text{Ar}]4s^23d^{10}$

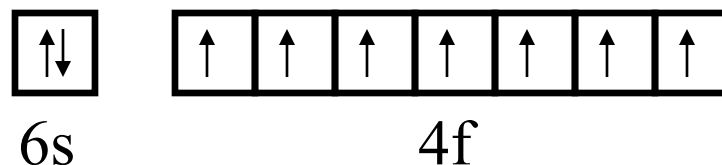


- for the *f* block metals, the principal energy level is two less than valence shell
 - ✓ two less than the Period number they really belong to
 - ✓ sometimes *d* electron in configuration

Eu

$Z = 63$, Period 6

$[\text{Xe}]6s^24f^7$



LECTURE QUIZ #15B on Electron Configuration

- 1) Write the full electron configuration for Fe/Co/Ni.
- 2) Write the shorthand configuration for Fe/Co/Ni and circle the valence electrons?

Lanthanides and Actinides

- The elements which fill the f orbitals have special names as a portion of a period, not as a group.
- The **lanthanide elements** (atomic numbers 57 to 70) have electrons entering the $4f$ sublevel.
- The **actinide elements** (including Uranium, at. no. 92, and Plutonium, at. no. 94) have electrons entering the $5f$ sublevel.

Electron configuration: transition and inner-transition Elements.

In general we use the Aufbau (or building up) principle to determine electron configuration, but as with most chemistry, there are exceptions to the rule. Look to the right.

Unfortunately, the Aufbau rule cannot predict all electron configuration as it doesn't take into account electron-electron interactions and other quantum mechanical effects. In the end the Aufbau is only a rule of thumb. Electronic levels have to be found using quantum calculations taking into account electron-electron interactions (not to mention spin orbit coupling).

Chromium	[Ar] 3d ⁵ 4s ¹
Copper	[Ar] 3d ¹⁰ 4s ¹
Niobium	[Kr] 4d ⁵ 5s ¹
Molybdenum	[Kr] 4d ⁵ 5s ¹
Ruthenium	[Kr] 4d ⁷ 5s ¹
Rhodium	[Kr] 4d ⁸ 5s ¹
Palladium	[Kr] 4d ¹⁰ 5s ⁰
Silver	[Kr] 4d ¹⁰ 5s ¹
Lanthanum	[Xe] 5d ¹ 6s ²
Cerium	[Xe] 4f ¹ 5d ¹ 6s ²
Gadolinium	[Xe] 4f ⁷ 5d ¹ 6s ²
Platinum	[Xe] 4f ¹⁴ 5d ⁹ 6s ¹
Gold	[Xe] 4f ¹⁴ 5d ¹⁰ 6s ¹
Actinium	[Rn] 6d ¹ 7s ²
Thorium	[Rn] 6d ² 7s ²
Protactinium	[Rn] 5f ² 6d ¹ 7s ²
Uranium	[Rn] 5f ³ 6d ¹ 7s ²
Neptunium	[Rn] 5f ⁴ 6d ¹ 7s ²
Curium	[Rn] 5f ⁷ 6d ¹ 7s ²

Practice – Use the Periodic Table to write the short electron configuration and orbital diagram for each of the following

- Na (at. no. 11)
- Te (at. no. 52)
- Tc (at. no. 43)

Practice – Use the Periodic Table to write the short electron configuration and orbital diagram for each of the following

- Na (at. no. 11) $[\text{Ne}]3s^1$

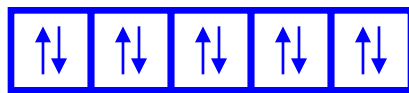


3s

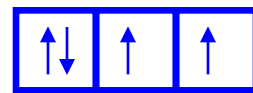
- Te (at. no. 52) $[\text{Kr}]5s^24d^{10}5p^4$



5s



4d

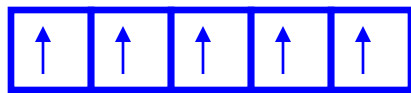


5p

- Tc (at. no. 43) $[\text{Kr}]5s^24d^5$



5s



4d

HOME PRACTICE PROBLEMS

1. Determine the ground-state electron configuration for each of the following elements:



sulfur



polonium

2. Predict the number of valence electrons present in each of the following atoms (include the outermost *d*-electrons when necessary):

29 total

A. B 3

B. Ba 2

C. Bi 3inp 2ins & 10ind 14inf

5 true valence & 24 pseudo

3. Determine the ground-state electron configuration for each of the following ions:

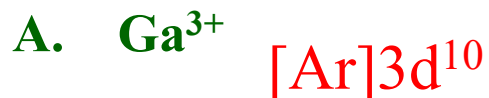


4. Predict the number of valence electrons present for each of the following ions:

A. In^{+} 2 true or 12 total

B. Tc^{+2} 5

5. Give the ground-state electron configuration and number of unpaired electrons expected for each of the following ions:



6. For each of the following ground-state ions, predict the type of orbital that the electrons of highest energy will occupy:

A. Fe^{+2} d

B. Bi^{+3} 6s 5d 4f