Chapter 7

Quantum Theory and the Electronic Structure of Atoms

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Wave properties and equations

(λ, υ, E)

$c = \lambda \times \nu$

$E = hc/\lambda$

Calculate the Energy of the electron in principal energy level

$$E_n = -R_H\left(\frac{1}{n^2}\right)$$

Calculate the Energy emitted or absorbed

$$\Delta E = R_H\left[\frac{1}{n^2_{\;i}} - \frac{1}{n^2_{\;f}}\right]$$

Quantum Numbers

(n, l, m_l, m_s)

Electron Configuration:

Aufbau Principle

Hund's Rule

Pauli Exclusion Principal

What is the wavelength of radiation (in nm) that has a frequency of $9.0 \times 10^{13}\ s^{-1}$ (Hz)? ($c = 3 \times 10^8$ m/s)

$$c = \lambda \times \nu$$

$$3\times10^8 \text{ m/s} = \lambda \times 9.0 \times 10^{13}\ s^{-1}$$

$$\lambda = \frac{3\times10^8}{9.0\times10^{13}}$$

$$\lambda = 3.33 \times 10^{-6}\text{m}$$

$$\lambda = 3.33 \times 10^{-6} \times 10^{9} = 3.33 \times 10^{3}\text{nm}$$

Calculate the frequency of visible light having a wavelength of 699 nm?

$$c = \lambda \text{ x } \nu$$

$$\nu = \frac{3\times10^{8}}{6.99\times10^{-7}}$$

$$\nu = 4.3 \times 10^{14}\ s^{-1}$$

What is the energy in joules of one photon of UV radiation with a wavelength 10 nm? ($c = 3 \times 10^8$ m/s; $h = 6.626 \times 10^{-34}$ J.s)

$$E = hc/\lambda$$

$$E = 3\times10^8 \times 6.626 \times 10^{-34}/1 \times 10^{-8}$$

$$E = 1.98 \times 10^{-17}\ \mathrm{J}$$

What is the energy of electron state in level with n=4 ?

$$E_n = -R_H\left(\frac{1}{n^2}\right)$$

$$E_n = -2.18x10^{-18}\left(\frac{1}{4^2}\right)$$

$$E_n = -1.36x10^{-19}\ \mathrm{J}$$

What is a likely energy level for a hydrogen atom with E_n= -6.053 X 10^{-20} J?
(constant R_H= 2.179 X 10^{-18} J)

$$E_n = -R_H(\frac{1}{n^2})$$

$n^2 = -R_H / E_n$

n^2 = (-2.179 X 10^{-18} J)/(-6.053 X 10^{-20} J)

n^2 = 35.999

n = 6

Because the value of n is an integer, 6 is the likely energy level of this photon.

The electron in a hydrogen atom is in the n = 2 state. When it drops to the ground state a photon is emitted. What is the wavelength of the photon?

$$\Delta E = R_H \left[\frac{1}{n^2{}_i} - \frac{1}{n^2{}_f}\right]$$

$$\Delta E = 2.18 \times 10^{-18} J \left[\frac{1}{2^2} - \frac{1}{1^2}\right]$$

$$\Delta E = -1.632 \times 10^{-18} \text{ J}$$

$$E = hc/\lambda$$

$$\lambda = hc/E = 6.63 \times 10^{-34} * 3 \times 10^{8} / 1.632 \times 10^{-18}$$

$$\lambda = 1.22 \times 10^{-7} \text{ m} = 122 \text{ nm}$$

How much energy must the atom absorb to move an electron from n =1 to n = 5?

$$\Delta E = R_H \left[\frac{1}{n^2_{\;i}} - \frac{1}{n^2_{\;f}}\right]$$

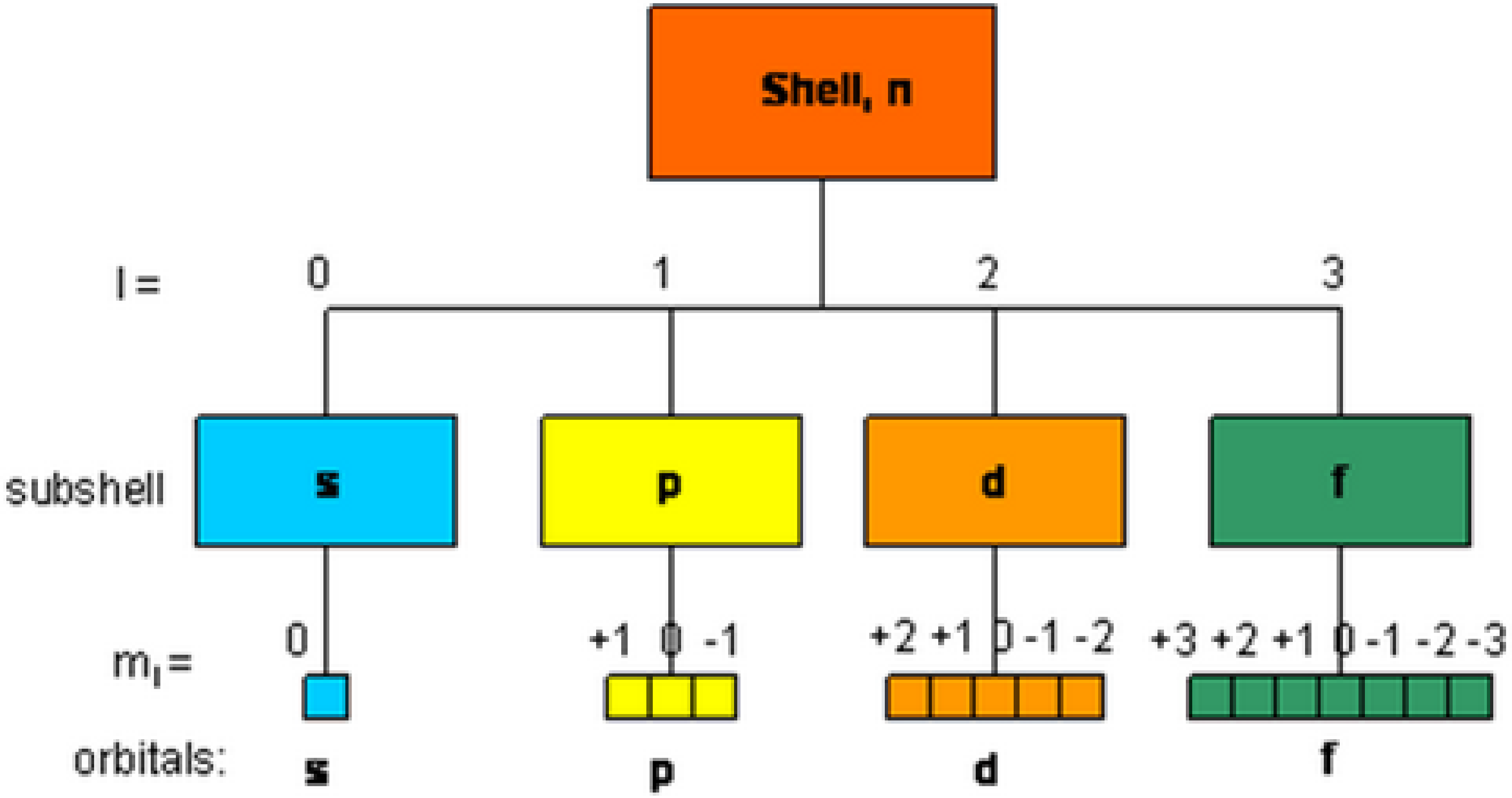
$$\Delta E = 2.18 \times 10^{-18}\, J \left[\frac{1}{1^2} - \frac{1}{5^2}\right]$$

ΔE= 2.093 x 10^{-18} J

Quantum Numbers

Name	Symbol	Allowed Values	Property
Principal	n	positive integers 1,2,3…	Orbital size and energy level
Secondary (Angular momentum)	*l*	Integers from 0 to (n-1)	Orbital shape (sublevels/subshells)
Magnetic	m_l	Integers –*l* to +*l*	Orbital orientation
Spin	m_s	+½ or –½	Electron spin Direction

Quantum Numbers



How many orbitals are in (n=4)	How many orbitals are in (l =3)	How many electron are (n=2)
For certain value of (n) there are **(n^2)** No. of orbitals	For certain value of (l) there are **(2 l +1)** No. of orbitals	For certain value of (n) there are **($2n^2$)** No. of electrons
4^2= 16 orbitals	$2 \times 3 + 1 = 7$ orbitals	2×2^2= 8 electrons

List the values of n, l, m_l, for orbitals in the 3d subshell

n=3 l=2 ml= -2,-1,0,1,2

List the values of n, l, m_l, for orbitals in the 2S subshell

n=2 l=0 ml= 0

List the values of l in n=3.

l =0,1,2

List the values of m_l in l=1.

m_l= -1, 0,1

Which one of the following sets of quantum numbers is not possible?

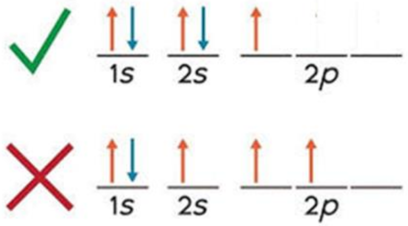
	n	l	m_l	m_s
A)	1	0	0	+½
B)	2	0	0	-½
C)	3	2	-2	-½
D)	2	0	1	+½

What is the maximum number of electrons in an atom that can have the following set of quantum numbers?

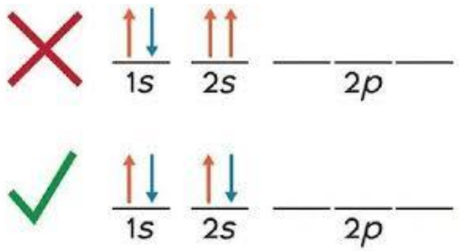
$n = 3 \quad l = 2 \quad ml = -2 \quad ms = +1/2$

Answer: 1

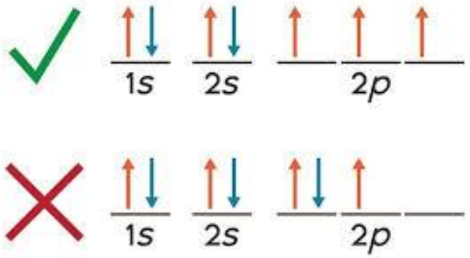
Filling Rules for Electron Orbitals



Aufbau Principle: Electrons are added one at a time to the lowest energy orbitals available until all the electrons of the atom have been accounted for.



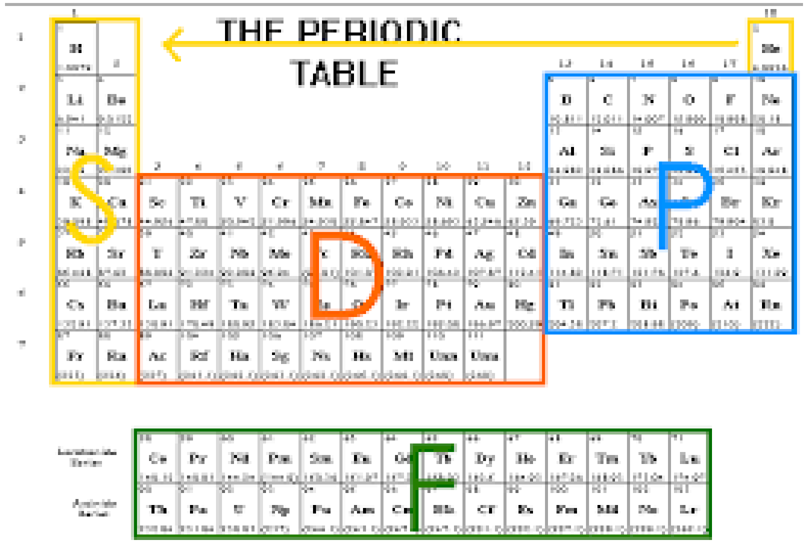
Pauli Exclusion Principle: An orbital can hold a maximum of two electrons. To occupy the same orbital, two electrons must spin in opposite directions.

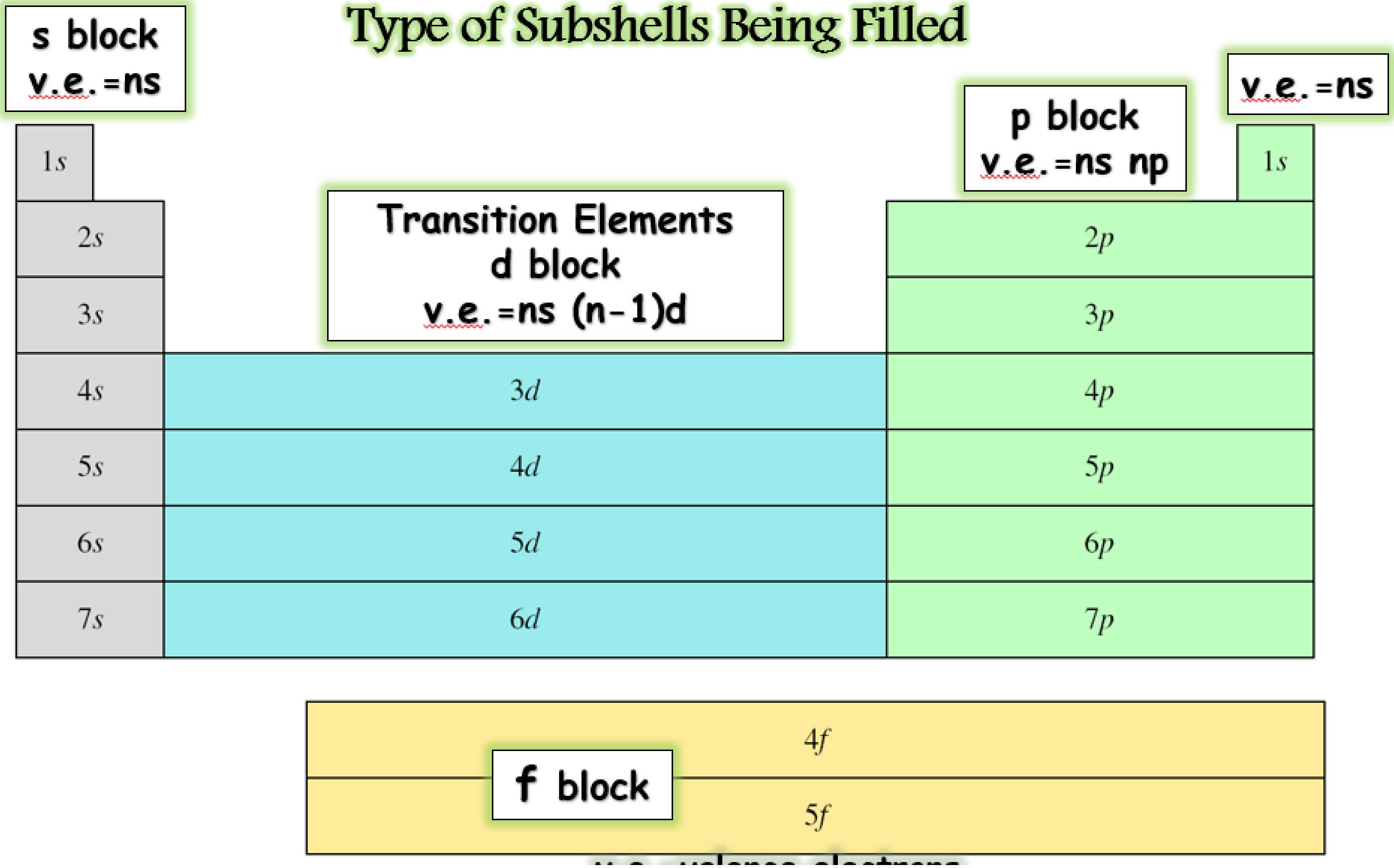


Hund's Rule: Electrons occupy equal-energy orbitals so that a maximum number of unpaired electrons results.

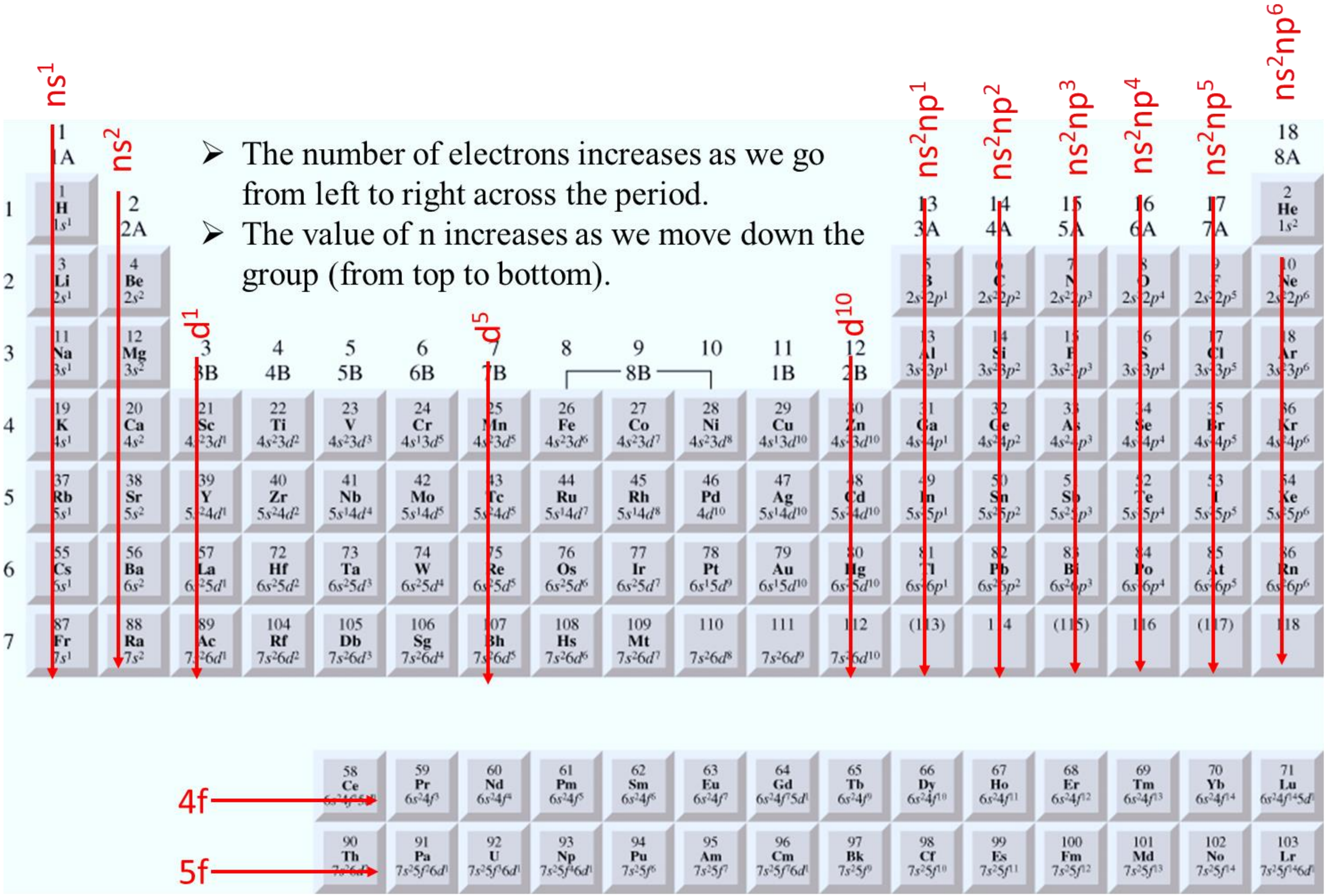
**Aufbau* is German for "building up"

Classification of Elements According to the Type of Subshells Being Filled





- ➢ The number of electrons increases as we go from left to right across the period.
- ➢ The value of n increases as we move down the group (from top to bottom).



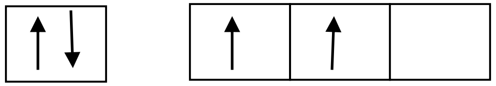
What is the electron configuration of Si?

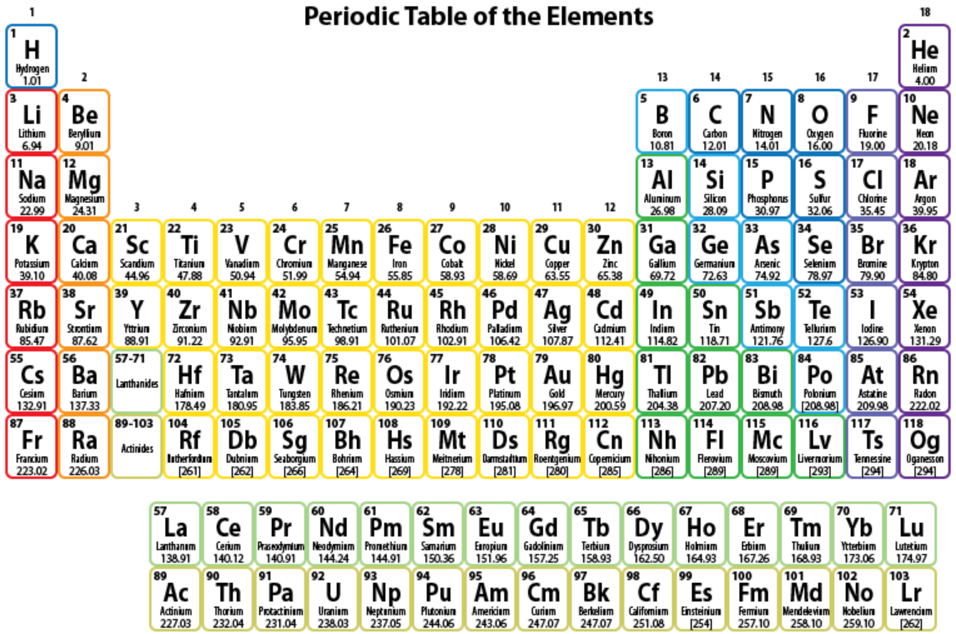
From the periodic table $\rightarrow$ 14 e

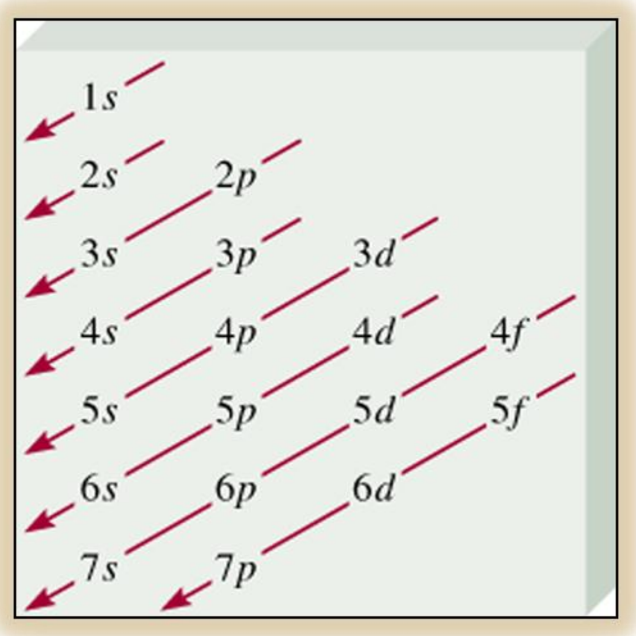
$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$

(OR)

[Ne] $3s^2\ 3p^2$







What is the electron configuration of Mo?

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

d orbital exception (The Stability of Half Filled & Filled d Orbitals)

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

$[Kr]\ 5s^1\ 4d^5$

Determine the group , period and the block of the following

^{12}Mg

$1s^2\ 2s^2\ 2p^6\ 3s^2$

Period **3**

group **2A (alkaline earth metal)**

block S, representative element (main group elements)

Determine the group , period and the block of the following

^{27}Co

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \underline{\mathbf{4s^2\ 3d^7}}$

Period **4**

group (2+7) 9B

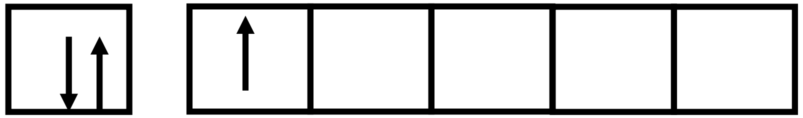
block d, Transition element

How many unpaired electrons does Sc (scandium) have? Is it paramagnetic or diamagnetic ?

$Sc \rightarrow 21e$

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \ 4s^2\ 3d^1$

$[Ar]4s^2\ 3d^1$



1 unpaired electron $\quad\therefore$ paramagnetic

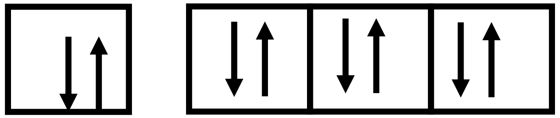
How many unpaired electrons does Na^+ have? Is it paramagnetic or diamagnetic ?

$Na \rightarrow 11e$

$1s^2\ 2s^2\ 2p^6\ 3s^1$

$Na^+ \rightarrow 10e$

$1s^2\ 2s^2\ 2p^6\ \cancel{3s^0}$



No unpaired electron $\quad \therefore$ diamagnetic

How many unpaired electrons does Fe^{2+} have? Is it paramagnetic or diamagnetic ?

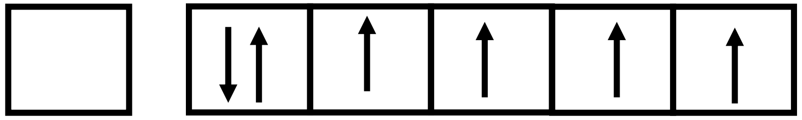
$Fe \rightarrow 26\ e$

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6$

$[Ar]4s^2\ 3d^6$

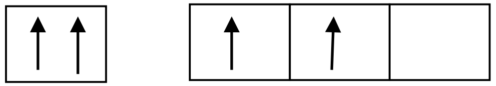
$Fe^{2+} \rightarrow 24\ e$

$[Ar]\cancel{4s^0}\ 3d^6$

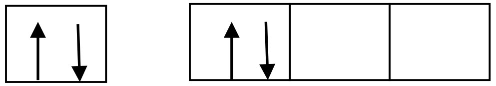


4 unpaired electron $\therefore$ Paramagnetic

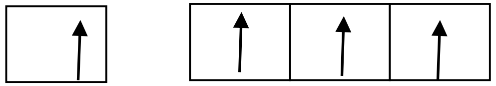
Which diagram **show a violation (break)** Aufbau principle, Hund's rule or Pauli exclusion principle?



Pauli exclusion principle



Hund's rule



Aufbau principle (building up)