

Chapter 7

Quantum Theory and the Electronic Structure of Atoms

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04/11/2018

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Quantum Theory and the Electronic Structure of Atoms

Wave
properties and
equations

$$(\lambda, \nu, E)$$

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

$$E = \frac{hc}{\lambda}$$

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

$$\Delta E = R_H \left[\frac{1}{n_i^2} - \frac{1}{n_f^2} \right]$$

Quantum
Numbers
(n, l, m_l, m_s)

Electron
Configuration:

Aufbau
Principle

Hund's Rule

Pauli Exclusion
Principle

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

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

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

$$\lambda = \frac{3 \times 10^8}{9.0 \times 10^{13}}$$

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

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

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

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

$$\nu = \frac{3 \times 10^8}{6.99 \times 10^{-7}}$$

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

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)

$$E = hc/\lambda$$

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

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

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

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

$$E_n = -2.18 \times 10^{-18} \left(\frac{1}{4^2} \right)$$

$$E_n = -1.36 \times 10^{-19} \text{ J}$$

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

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

$$n^2 = -R_H / E_n$$

$$n^2 = (-2.179 \times 10^{-18} \text{ J}) / (-6.053 \times 10^{-20} \text{ J})$$

$$n^2 = 35.999$$

$$n = 6$$

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?

$$\Delta E = R_H \left[\frac{1}{n_i^2} - \frac{1}{n_f^2} \right]$$

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

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

$$E = hc/\lambda$$

$$\lambda = hc/E = 6.63 \times 10^{-34} \text{ m} \cdot \text{s} \cdot 3 \times 10^8 \text{ s}^{-1} / 1.632 \times 10^{-18} \text{ J}$$

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

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

$$\Delta E = R_H \left[\frac{1}{n_i^2} - \frac{1}{n_f^2} \right]$$

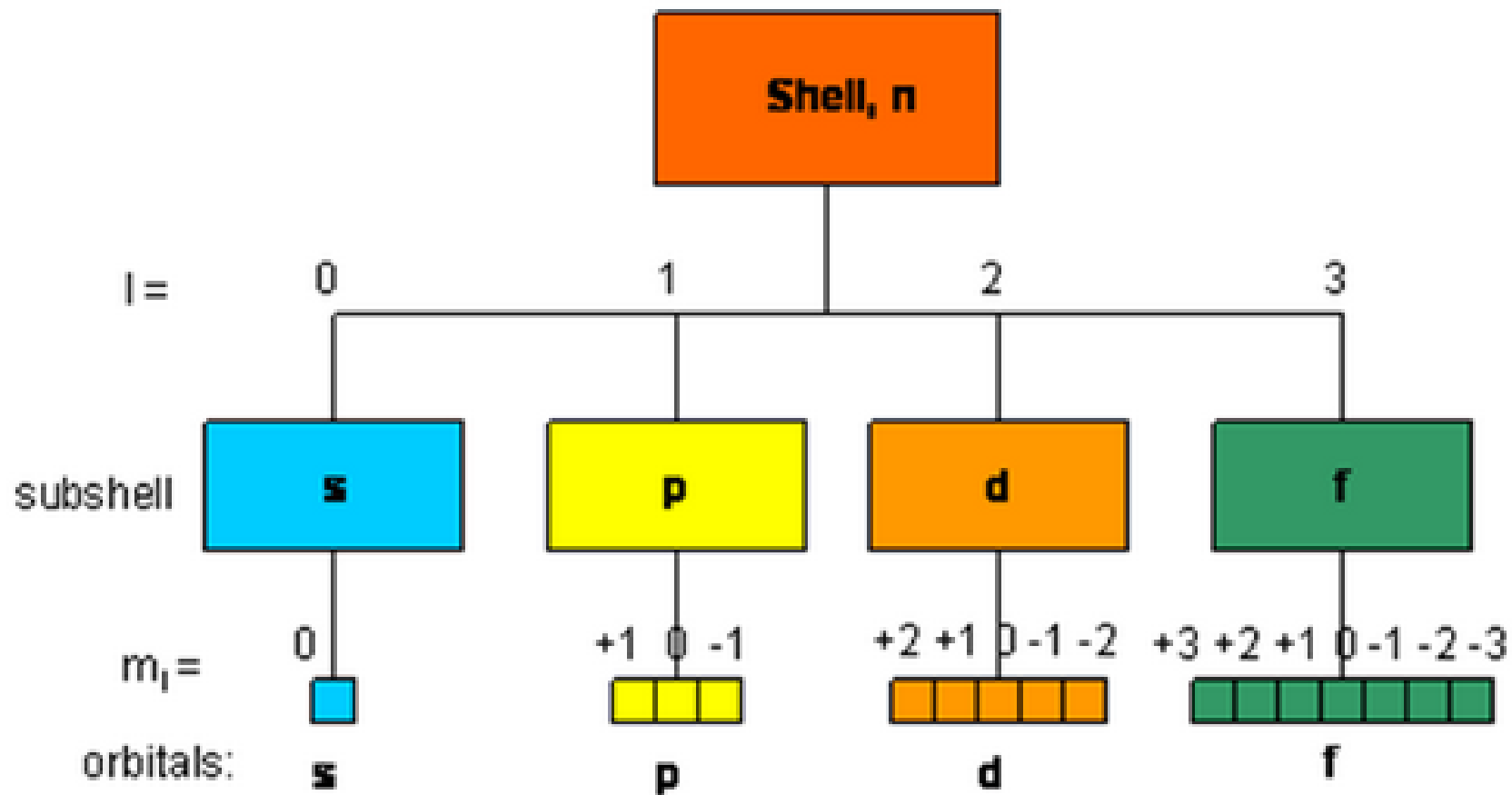
$$\Delta E = 2.18 \times 10^{-18} \text{ J} \left[\frac{1}{1^2} - \frac{1}{5^2} \right]$$

$$\Delta E = 2.093 \times 10^{-18} \text{ J}$$

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	$+1/2$ or $-1/2$	Electron spin Direction

Quantum Numbers



<p>How many orbitals are in (n=4)</p>	<p>How many orbitals are in (l =3)</p>	<p>How many electron are (n=2)</p>
<p>For certain value of (n) there are (n²) No. of orbitals</p>	<p>For certain value of (l) there are (2 l +1) No. of orbitals</p>	<p>For certain value of (n) there are (2n²) No. of electrons</p>
<p>4²= 16 orbitals</p>	<p>2 × 3 + 1 = 7 orbitals</p>	<p>2 × 2²= 8 electrons</p>

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

$n=3$ $l=2$ $m_l = -2, -1, 0, 1, 2$

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

$n=2$ $l=0$ $m_l = 0$

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	$+1/2$
B)	2	0	0	$-1/2$
C)	3	2	-2	$-1/2$
D)	2	0	1	$+1/2$

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

$$n = 3 \quad l = 2 \quad m_l = -2 \quad m_s = +1/2$$

Answer: 1

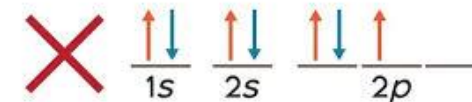
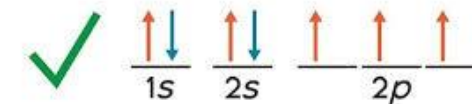
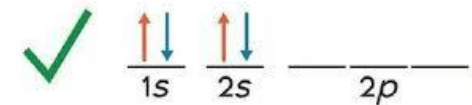
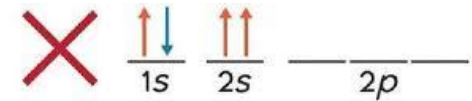
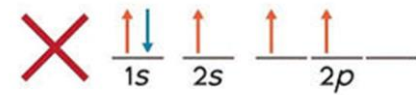
Filling Rules for Electron Orbitals

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"

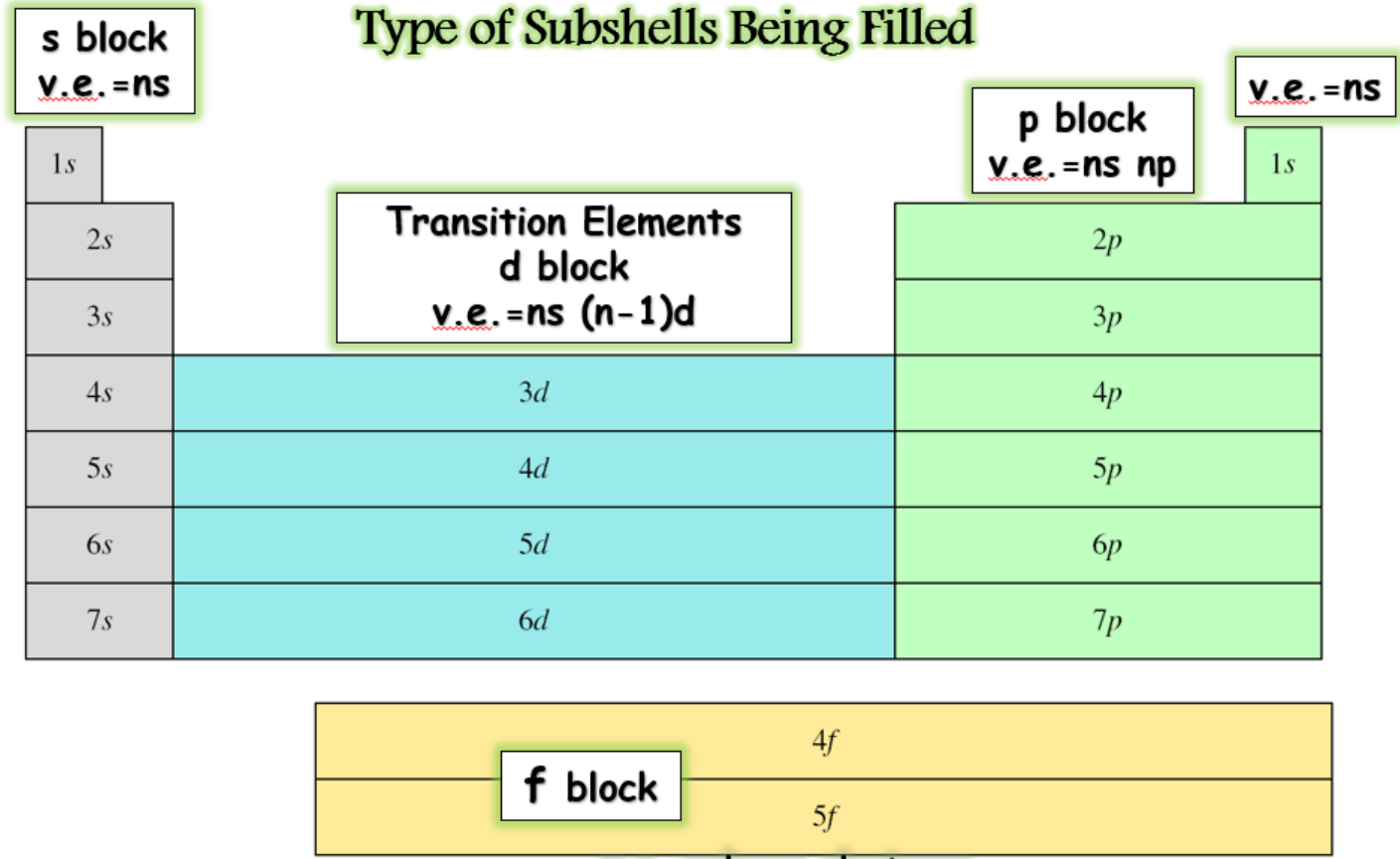


Classification of Elements According to the Type of Subshells Being Filled

THE PERIODIC TABLE

The periodic table is divided into four main blocks based on the type of subshell being filled:

- s block:** Elements in groups 1 and 2, plus Helium (He).
- p block:** Elements in groups 13 through 18.
- d block:** Transition elements in groups 3 through 10.
- f block:** Lanthanide and actinide series.



... valence electrons

ns^1 ns^2 d^1 d^5 d^{10} ns^2np^1 ns^2np^2 ns^2np^3 ns^2np^4 ns^2np^5 ns^2np^6

1 A 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
 8A
 1 H 2 He
 $1s^1$ $1s^2$
 2 3 4
 Li Be
 $2s^1$ $2s^2$
 3 4 5 6 7 8 9 10 11 12
 Na Mg B C N O F Ne
 $3s^1$ $3s^2$ $3s^23p^1$ $3s^23p^2$ $3s^23p^3$ $3s^23p^4$ $3s^23p^5$ $3s^23p^6$
 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
 K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
 $4s^1$ $4s^2$ $4s^23d^1$ $4s^23d^2$ $4s^23d^3$ $4s^13d^5$ $4s^23d^5$ $4s^23d^6$ $4s^23d^7$ $4s^23d^8$ $4s^13d^{10}$ $4s^23d^{10}$ $4s^24p^1$ $4s^24p^2$ $4s^24p^3$ $4s^24p^4$ $4s^24p^5$ $4s^24p^6$
 5 6 7 8 9 10 11 12 13 14 15 16 17 18
 Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe
 $5s^1$ $5s^2$ $5s^24d^1$ $5s^24d^2$ $5s^14d^4$ $5s^14d^5$ $5s^24d^5$ $5s^14d^7$ $5s^14d^8$ $4d^{10}$ $5s^14d^{10}$ $5s^24d^{10}$ $5s^25p^1$ $5s^25p^2$ $5s^25p^3$ $5s^25p^4$ $5s^25p^5$ $5s^25p^6$
 6 7 8 9 10 11 12 13 14 15 16 17 18
 Cs Ba La Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn
 $6s^1$ $6s^2$ $6s^25d^1$ $6s^25d^2$ $6s^25d^3$ $6s^25d^4$ $6s^25d^5$ $6s^25d^6$ $6s^25d^7$ $6s^15d^9$ $6s^15d^{10}$ $6s^25d^{10}$ $6s^26p^1$ $6s^26p^2$ $6s^26p^3$ $6s^26p^4$ $6s^26p^5$ $6s^26p^6$
 7 8 9 10 11 12 13 14 15 16 17 18
 Fr Ra Ac Rf Db Sg Bh Hs Mt Nih Nh Fl Ogh Lv Ten
 $7s^1$ $7s^2$ $7s^26d^1$ $7s^26d^2$ $7s^26d^3$ $7s^26d^4$ $7s^26d^5$ $7s^26d^6$ $7s^26d^7$ $7s^26d^8$ $7s^26d^9$ $7s^26d^{10}$ (113) 114 (115) 116 (117) 118

$4f$ $5f$

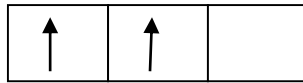
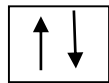
58 Ce $6s^24f^58s^2$ 59 Pr $6s^24f^3$ 60 Nd $6s^24f^4$ 61 Pm $6s^24f^5$ 62 Sm $6s^24f^6$ 63 Eu $6s^24f^7$ 64 Gd $6s^24f^75d^1$ 65 Tb $6s^24f^9$ 66 Dy $6s^24f^{10}$ 67 Ho $6s^24f^{11}$ 68 Er $6s^24f^{12}$ 69 Tm $6s^24f^{13}$ 70 Yb $6s^24f^{14}$ 71 Lu $6s^24f^{14}5d^1$
 90 Th $7s^26d^2$ 91 Pa $7s^25f^6d^1$ 92 U $7s^25f^6d^1$ 93 Np $7s^25f^6d^1$ 94 Pu $7s^25f^6$ 95 Am $7s^25f^7$ 96 Cm $7s^25f^76d^1$ 97 Bk $7s^25f^9$ 98 Cf $7s^25f^{10}$ 99 Es $7s^25f^{11}$ 100 Fm $7s^25f^{12}$ 101 Md $7s^25f^{13}$ 102 No $7s^25f^{14}$ 103 Lr $7s^25f^{14}6d^1$

What is the electron configuration of Si?

From the periodic table → 14 e

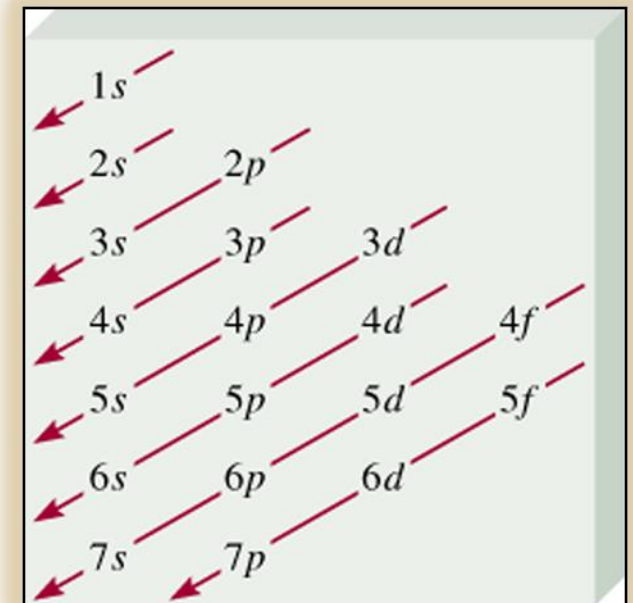


(OR)

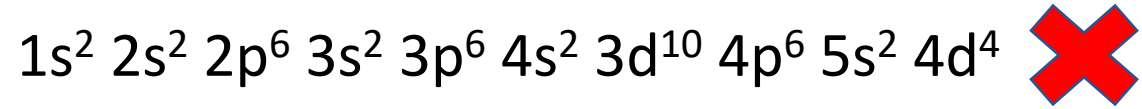


Periodic Table of the Elements

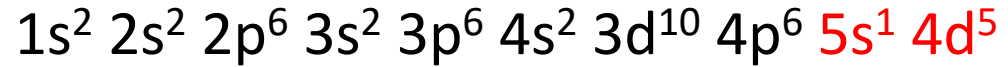
1 H Hydrogen 1.01	2 He Helium 4.00											13 B Boron 10.81	14 C Carbon 12.01	15 N Nitrogen 14.01	16 O Oxygen 16.00	17 F Fluorine 19.00	18 Ne Neon 20.18
3 Li Lithium 6.94	4 Be Beryllium 9.01											13 Al Aluminum 26.98	14 Si Silicon 28.09	15 P Phosphorus 30.97	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Ar Argon 39.95
11 Na Sodium 22.99	12 Mg Magnesium 24.31											13 Ga Gallium 69.72	14 Ge Germanium 72.63	15 As Arsenic 74.92	16 Se Selenium 78.97	17 Br Bromine 79.90	18 Kr Krypton 84.90
19 K Potassium 39.10	20 Ca Calcium 40.08	21 Sc Scandium 44.96	22 Ti Titanium 47.88	23 V Vanadium 50.94	24 Cr Chromium 51.99	25 Mn Manganese 54.94	26 Fe Iron 55.85	27 Co Cobalt 58.93	28 Ni Nickel 58.69	29 Cu Copper 63.55	30 Zn Zinc 65.38	31 In Indium 114.82	32 Sn Tin 118.71	33 Sb Antimony 121.76	34 Te Tellurium 127.6	35 I Iodine 126.90	36 Xe Xenon 131.29
37 Rb Rubidium 85.47	38 Sr Strontium 87.62	39 Y Yttrium 88.91	40 Zr Zirconium 91.22	41 Nb Niobium 92.91	42 Mo Molybdenum 95.95	43 Tc Technetium 98.91	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Palladium 106.42	47 Ag Silver 107.87	48 Cd Cadmium 112.41	49 Tl Thallium 204.38	50 Pb Lead 207.2	51 Bi Bismuth 208.98	52 Po Polonium [209]	53 At Astatine [209]	54 Rn Radon [222]
55 Cs Cesium 132.91	56 Ba Barium 137.33	57-71 Lanthanides	72 Hf Hafnium 178.49	73 Ta Tantalum 180.95	74 W Tungsten 183.85	75 Re Rhenium 186.21	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.97	80 Hg Mercury 200.59	81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.98	84 Po Polonium [209]	85 At Astatine [209]	86 Rn Radon [222]
87 Fr Francium [223]	88 Ra Radium [226]	89-103 Actinides	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [278]	110 Ds Darmstadtium [281]	111 Rg Roentgenium [289]	112 Cn Copernicium [285]	113 Nh Nihonium [286]	114 Fl Flerovium [289]	115 Mc Moscovium [289]	116 Lv Livermorium [293]	117 Ts Tennessine [294]	118 Og Oganesson [294]
57 La Lanthanum 138.91	58 Ce Cerium 140.12	59 Pr Praseodymium 140.91	60 Nd Neodymium 144.24	61 Pm Promethium 144.91	62 Sm Samarium 150.36	63 Eu Europium 151.96	64 Gd Gadolinium 157.25	65 Tb Terbium 158.93	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93	68 Er Erbium 167.26	69 Tm Thulium 168.93	70 Yb Ytterbium 173.06	71 Lu Lutetium 174.97			
89 Ac Actinium 227.03	90 Th Thorium 232.04	91 Pa Protactinium 231.04	92 U Uranium 238.03	93 Np Neptunium 237.05	94 Pu Plutonium 244.06	95 Am Americium 243.06	96 Cm Curium 247.07	97 Bk Berkelium 247.07	98 Cf Californium 251.08	99 Es Einsteinium [254]	100 Fm Fermium 257.10	101 Md Mendelevium 258.10	102 No Nobelium 259.10	103 Lr Lawrencium [262]			



What is the electron configuration of Mo?



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



Determine the group , period and the block of the following

^{12}Mg

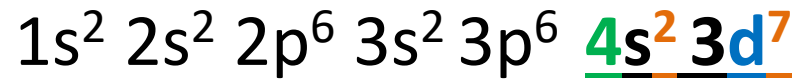
$1s^2 2s^2 2p^6 3s^2$

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



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

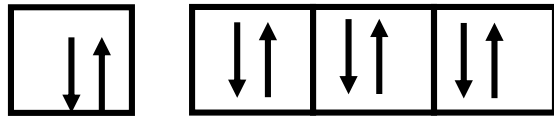
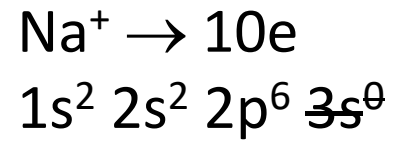
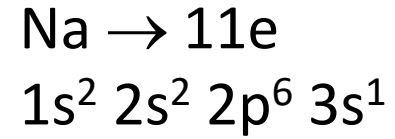
$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$

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



1 unpaired electron \therefore paramagnetic

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



No unpaired electron \therefore diamagnetic

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

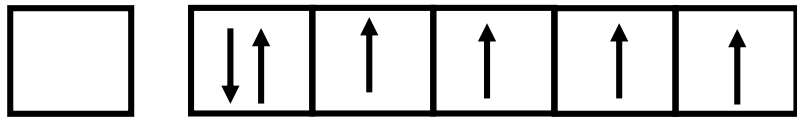
$\text{Fe} \rightarrow 26 \text{ e}$

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

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

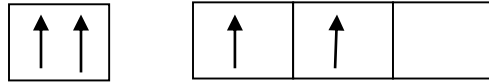
$\text{Fe}^{2+} \rightarrow 24 \text{ e}$

$[\text{Ar}]~~4s~~ 3d^6$

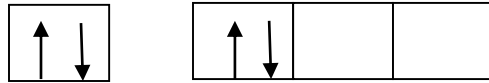


4 unpaired electron \therefore Paramagnetic

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)