

Chapter 8: Electron Configuration + Periodicity

Electron Configuration of Atoms - basis for explaining the behavior of elements in periodic table.

Nomenclature: $_$ atomic orbital
 \uparrow unpaired electron
 $\uparrow\downarrow$ spin paired electrons

Note: The Pauli Exclusion Principle says that $\uparrow\uparrow$ is impossible.

First Period (1st horizontal row) of Periodic Table: $n=1$

	1s	Notation	Recall: for a neutral atom, the atomic number (# protons) = # electrons
${}_1\text{H}$	\uparrow	$1s^1$	
${}_2\text{He}$	$\uparrow\downarrow$	$1s^2$	He is a very stable element - noble gas. $n=1$ energy level filled

Second Period (2nd horizontal row) of Periodic Table: $n=2$

	1s	2s	2p			Shorthand Notation
${}_3\text{Li}$	$\uparrow\downarrow$	\uparrow	$_$	$_$	$_$	$1s^2 2s^1$
${}_4\text{Be}$	$\uparrow\downarrow$	$\uparrow\downarrow$	$_$	$_$	$_$	$1s^2 2s^2$
${}_5\text{B}$	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow	$_$	$_$	$1s^2 2s^2 2p^1$
${}_6\text{C}$	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow	\uparrow	$_$	$1s^2 2s^2 2p^2$
${}_7\text{N}$	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow	\uparrow	\uparrow	$1s^2 2s^2 2p^3$ or $1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1$
${}_8\text{O}$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow	\uparrow	$1s^2 2s^2 2p^4$
${}_9\text{F}$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	\uparrow	$1s^2 2s^2 2p^5$
${}_{10}\text{Ne}$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$1s^2 2s^2 2p^6$

$\# e^- = 2n^2 = 8$

very stable
 $n=1, n=2$ energy levels filled

We used Hund's Rule: electrons must occupy all the orbitals of a given sublevel singly before pairing begins.

diamagnetic: refers to an atom in which the electrons are all paired up

examples: ${}_2\text{He}$, ${}_4\text{Be}$, ${}_{10}\text{Ne}$

paramagnetic: refers to an atom in which there are unpaired electrons.

examples: ${}_5\text{B}$, ${}_9\text{F}$ (1 unpaired e^-) ${}_7\text{N}$ (3 unpaired e^-) - exhibits paramagnetism to greatest extent.
 ${}_6\text{C}$ (2 unpaired e^-)

Third Period (3rd horizontal row) of Periodic Table: $n=3$

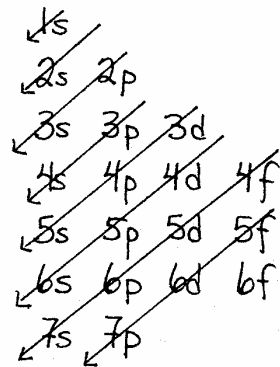
	10e ⁻	3s	3p			Shorthand Notation
11 Na	[Ne]	↑	—	—	—	[Ne] 3s ¹ or 1s ² 2s ² 2p ⁶ 3s ¹
12 Mg	[Ne]	↑↓	—	—	—	[Ne] 3s ²
13 Al	[Ne]	↑↓	↑	—	—	[Ne] 3s ² 3p ¹
14 Si	[Ne]	↑↓	↑	↑	—	[Ne] 3s ² 3p ²
15 P	[Ne]	↑↓	↑	↑	↑	[Ne] 3s ² 3p ³
16 S	[Ne]	↑↓	↑↓	↑	↑	[Ne] 3s ² 3p ⁴
17 Cl	[Ne]	↑↓	↑↓	↑↓	↑	[Ne] 3s ² 3p ⁵
18 Ar	[Ne]	↑↓	↑↓	↑↓	↑↓	[Ne] 3s ² 3p ⁶ very stable

Fourth Period (4th horizontal Row) of Periodic Table: $n=4$

	18e ⁻	3d					4s	4p		
19 K	[Ar]	—	—	—	—	—	↑	—	—	—
20 Ca		—	—	—	—	—	↑↓	—	—	—
21 Sc		↑	—	—	—	—	↑↓	—	—	—
22 Ti		↑	↑	—	—	—	↑↓	—	—	—
23 V		↑	↑	↑	—	—	↑↓	—	—	—
* 24 Cr		↑	↑	↑	↑	↑	↑	—	—	—
25 Mn		↑	↑	↑	↑	↑	↑↓	—	—	—
26 Fe		↑↓	↑	↑	↑	↑	↑↓	—	—	—
27 Co		↑↓	↑↓	↑	↑	↑	↑↓	—	—	—
28 Ni		↑↓	↑↓	↑↓	↑	↑	↑↓	—	—	—
* 29 Cu		↑↓	↑↓	↑↓	↑↓	↑↓	↑	—	—	—
30 Zn		↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	—	—	—
31 Ga		↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	—	—
32 Ge		↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	—
33 As		↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑
34 Se		↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑
35 Br		↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑
36 Kr		↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓

Exception to Filling Rule

What we saw was that the energy levels filled up differently than what we expected. One way to remember the general order is



Note: There are still exceptions to the filling order eg Cu & Cr. These two are the only ones you are responsible for.

Another way is to use the periodic table.

The periodic table has A groups and B groups. (vertical columns)

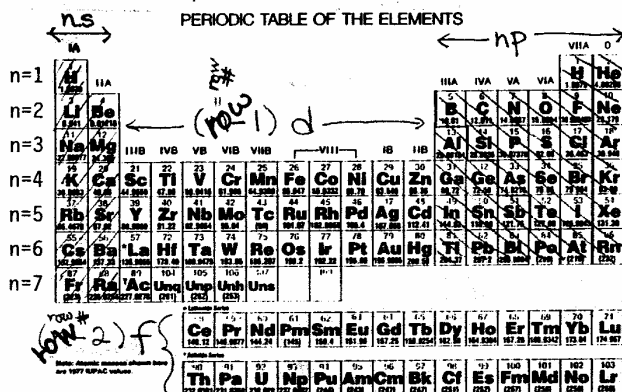
(Note: periodic tables can be different - use periodic table on sheet + in textbook)
 Periods are horizontal rows: 1st period corresponds to $n=1$ energy level etc.

A Group: s and p orbitals are being filled.

B Group: ns orbital is filled and $(n-1)$ d sublevel is being filled.

Exercise: Follow the elements in periodic table in order of increasing atomic number and state what orbitals are being filled. (Table 5-5) Figure 5-31

Example: In the fourth period ($n=4$), we first put electrons in 4s orbital, then electrons are placed in $n-1 = 4-1 = 3d$ sublevel in B groups. Finally electrons are put into 4p energy level.



ELECTRONIC CONFIGURATION OF THE ELEMENTS

There are two elements in the first period (row) of the periodic table, hydrogen and helium. The electrons in hydrogen and helium atoms occupy the 1s orbital.

There are eight elements (numbers 3-10) in the second period of the periodic table. The outermost electrons in these elements occupy the 2s and 2p orbitals; that is, they all have $n = 2$ where n is the outermost occupied energy level.

	1s	2s	2p	Outermost Configuration
1H	---	---	---	---
2He	---	---	---	---
3Li	---	---	---	---
4Be	---	---	---	---
5B	---	---	---	---
6C	---	---	---	---
7N	---	---	---	---
8O	---	---	---	---
9F	---	---	---	---
10Ne	---	---	---	---

There are also eight elements (numbers 11-18) in the third period. The outermost electrons in these elements occupy the 3s and 3p orbitals ($n = 3$).

	3s	3p
11Na	[Ne]	---
12Mg	[Ne]	---
13Al	[Ne]	---
14Si	[Ne]	---
15P	[Ne]	---
16S	[Ne]	---
17Cl	[Ne]	---
18Ar	[Ne]	---

The symbol for a noble gas indicates a number of electrons corresponding to the atomic number of the noble gas, in filled sets. [Ne] corresponds to 2 e⁻, and [Ar] corresponds to 18 e⁻ in filled sets of orbitals.

There are eighteen elements (numbers 19-36) in the fourth period of the periodic table. As we shall see, the electrons added in these elements occupy the 4s, 3d, and 4p orbitals. ($n = 4$)

	3d	4s	4p
19K [Ar]	---	---	---
20Ca	---	---	---
21Sc	---	---	---
22Ti	---	---	---
23V	---	---	---
24Cr	---	---	---
25Mn	---	---	---
26Fe	---	---	---
27Co	---	---	---
28Ni	---	---	---
29Cu	---	---	---
30Zn	---	---	---
31Ga	---	---	---
32Ge	---	---	---
33As	---	---	---
34Se	---	---	---
35Br	---	---	---
36Kr	---	---	---

[Ar] is not repeated if time. It is understood to be there

PERIODIC TABLE OF THE ELEMENTS

	1A	2A	3A	4A	5A	6A	7A	8A	9A	10A	11A	12A	13A	14A	15A	16A	17A	18A																	
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18																	
	H	He											Li	Be	B	C	N	O	F	Ne															
	Na	Mg	Al	Si	P	S	Cl	Ar	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr									
	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	Ra	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	
	Fr	Ra	Uuo	Uup	Uuq	Uur	Uus	Uut	Uuq	Uur	Uus	Uut	Uuq	Uur	Uus	Uut	Uuq	Uur	Uus	Uut	Uuq	Uur	Uus	Uut	Uuq	Uur	Uus	Uut	Uuq	Uur	Uus	Uut	Uuq	Uur	Uus

- 1s
- 2s 2p
- 3s 3p 3d
- 4s 4p 4d 4f
- 5s 5p 5d 5f
- 6s 6p 6d
- 7s 7p

The pattern for filling atomic orbitals has been evolved.

Summary on Order of Filling Atomic Orbitals

There are several mnemonic devices (including this one) to assist one in remembering the order in which electrons are "added" to atoms.

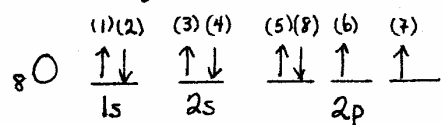
Source: Adapted, permission obtained from the 1977 IUPAC tables.

Example: In the sixth period ($n=6$), the 6s orbital is filled, then the energy sublevels are filled in the following order: 4f, 5d then 6p.

Relation Between Quantum Numbers and Electronic Configuration

Recall: every electron in an atom has its own unique set of 4 quantum numbers.

Example: Write a complete set of 4 quantum numbers for each electron in an oxygen atom, ${}_8\text{O}$. There are 8 electrons in ${}_8\text{O}$; there should be 8 sets of 4 quantum numbers, one for each electron.



Electron	n	l	m_l	m_s
1	1	0 (since is s orbital)	0	$+\frac{1}{2}$
2	1	0	0	$-\frac{1}{2}$
3	2	0 (since is s orbital)	0	$+\frac{1}{2}$
4	2	0	0	$-\frac{1}{2}$
5	2	1 (since is p orbital)	-1	$+\frac{1}{2}$
6	2	1	0	$+\frac{1}{2}$
7	2	1	+1	$+\frac{1}{2}$
8	2	1	-1	$-\frac{1}{2}$

Notes on bookkeeping: $\uparrow \equiv$ spin is $+\frac{1}{2}$
 $\downarrow \equiv$ spin is $-\frac{1}{2}$
 the 3 p orbitals are labelled $m_l = \underline{-1} \quad \underline{0} \quad \underline{+1}$

Example: What is an appropriate set of 4 quantum numbers for the last electron to go into an element of:

	n	l	m_l	m_s		n	l	m_l	m_s
(a) Na	3	0(s)	0	$\pm\frac{1}{2}$	(c) ${}_{82}\text{Pb}$	6	1(p)	-1, 0, +1	$\pm\frac{1}{2}$
(b) Ru	4	2(d)	-2, -1, 0, +1, +2	$\pm\frac{1}{2}$	(d) ${}_{77}\text{No}$	5	3(f)	-3, -2, -1, 0, +1, +2, +3	$\pm\frac{1}{2}$

Preview of Periodic Properties

The elements of a certain Group tend to behave similarly in chemical reactions because it is the OUTSIDE electrons (the electrons that are farthest from the nucleus) that are involved in chemical reactions. These are the outermost s and p electrons - called VALENCE electrons. The elements in a certain group all have the same number of valence electrons.

Group IA (H, Li, Na, K, ...) have 1 electron in outermost s orbital: ns^1
 Group IIA (Be, Mg, Ca, ...) have 2 electrons in outermost s orbital: ns^2
 Group VIA (O, S, Se, ...) have 6 electrons in outermost s + p orbitals: $ns^2 np^4$

Summarizing Example:

- The not-yet-discovered element with atomic number 115 falls into which periodic group?
- Its chemical behavior would be most similar to which elements?
- Its outer electrons would have what shorthand notation? How many valence e's?
- Its electron configuration is what? (use periodic table)
- An acceptable set of 4 quantum numbers for the last electron to be put into this element is ____.

ANS:

- VA
- N, P, As - other VA elements
- $7s^2 7p^3$; 5 valence electrons
- $[Rn] 5f^{14} 6d^{10} 7s^2 7p^3$
 $86e^-$

(c) $n=7$, $l=1$, m_l could be -1 or 0 or $+1$, m_s could be $+\frac{1}{2}$ or $-\frac{1}{2}$

Chemical Periodicity

We just finished discussing the structure of atoms and introduced its relationship to chemical periodicity: the variation in the properties of elements with their positions in the periodic table.

electron as wave-like \Rightarrow Schrodinger Equation \Rightarrow quantum numbers: n, l, m_l, m_s \Rightarrow electron configuration $1s^2 2s^2 2p^6 \dots$ \Rightarrow predicted properties (periodicity) according to periodic table

The history of the periodic table is given in the text ... Mendeleev and Meyer (1869) independently arranged the known elements into a pattern based on their properties, thus setting the stage for the ...

Periodic Law: The properties of the elements are periodic functions of their atomic numbers (the numbers of protons in the nucleus).

Terms for the Periodic Table:

group or family: vertical columns
the elements have similar chemical and physical properties.

period: horizontal rows
the elements have properties that change progressively across the table.

Group A: "representative" elements
show distinct and fairly regular variations in properties with the atomic number
their last electron is added to an s or p orbital

Group B: show less dramatic changes in properties with increasing atomic number
their last electron is added to an $(n-1)d$ orbital which lies inside the outer ns and np electrons.

The representative elements:

Group IA (except H)	alkali metals	ns^1
Group IIA	alkaline earth metals	ns^2
Group VIIA	halogens (salt-formers)	$ns^2 np^5$
Group 0	noble (rare) gases	$ns^2 np^6$ (except He)

d-transition elements: in B group (except IIB)

electrons are being added to d-orbitals

(Note: IIB is excluded since their last e^- is added to s orbital. Elements are Zn, Cd, Hg, but their properties are similar to d-transition elements.)

1st transition series: $_{21}\text{Sc} \rightarrow _{29}\text{Cu}$

2nd transition series: $_{39}\text{Y} \rightarrow _{47}\text{Ag}$

3rd transition series: $_{57}\text{La}, _{72}\text{Hf} \rightarrow _{79}\text{Au}$

4th transition series: $_{89}\text{Ac}$

inner transition elements: located between IIIB and IVB

electrons are being added to f orbitals

1st inner transition series: lanthanides $_{58}\text{Ce} \rightarrow _{71}\text{Lu}$ (lutetium)

2nd inner transition series: actinides $_{90}\text{Th} \rightarrow _{103}\text{Lr}$ (lawrencium)

Lewis Dot Representations of Representative Elements

- only the electrons shown in the outer s & p orbitals are shown as dots
These are called VALENCE electrons.
- paired and unpaired electrons are shown.

7-1
TABLE 5-3 Lewis Electron Dot Formulas for Representative Elements

GROUP	IA	IIA	IIIA	IVA	VA	VIA	VIIA	0
Number of Electrons in Outer Shell	1	2	3	4	5	6	7	8 (except He)
Row 1	H·							He:
Row 2	Li·	Be:	B·	C·	N·	O·	F·	Ne:
Row 3	Na·	Mg:	Al·	Si·	P·	S·	Cl·	Ar:
Row 4	K·	Ca:	Ga·	Ge·	As·	Se·	Br·	Kr:
Row 5	Rb·	Sr:	In·	Sn·	Sb·	Te·	I·	Xe:
Row 6	Cs·	Ba:	Tl·	Pb·	Bi·	Po·	At·	Rn:
Row 7	Fr·	Ra:						

Memorize or
deduce from
periodic table.

Periodic Properties for Group A Elements

The physical and chemical properties of elements recur periodically.

There are 5 properties we will consider in depth.

- | | |
|-----------------------|-----------------------|
| (1) atomic radii | (4) ionic radii |
| (2) ionization energy | (5) electronegativity |
| (3) electron affinity | |

(1) Atomic Radii

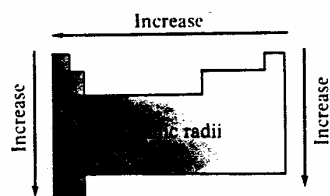
Values have been determined indirectly. (units : angstroms $1\text{\AA} = 10^{-10}\text{m}$
nanometers $1 \times 10^{-9}\text{m}$)

as we move from left to right within a particular energy level (eg $n=2$)

the atomic number increases. Therefore for a neutral atom, protons are added to the nucleus; ^{increasing the nuclear charge} electrons are added to the electron cloud in same major energy level. There is greater and greater attraction; the electron cloud is pulled closer and closer into the nucleus.

Result : the atomic radii decreases. Eg $\text{Li} > \text{Be} > \text{B} > \text{C} > \text{N} > \text{O} > \text{F} > \text{Ne}$

as we move from top ($n=1$) to bottom ($n=7$), electrons are added to higher and higher energy levels which are correspondingly larger and larger. Result : the atomic radii increases. Eg $\text{Be} < \text{Mg} < \text{Ca} < \text{Sr} < \text{Ba}$



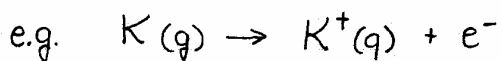
general trend in atomic radii of A group elements with position in periodic table.

Chemical reactions result from the interaction of the outermost electrons of the elements involved. Therefore it is important to know how tightly the electrons of an element are held and how easily the elements gain or lose electrons.

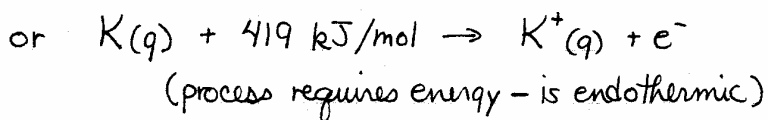
To give us this information, the energy involved in these processes is measured.

Convention : energy is released (exothermic) : energy has negative value
energy is absorbed (endothermic) : energy has positive value

(2) First Ionization Energy: minimum amount of energy required to remove the most loosely bound electron from an isolated gaseous atom to form an ion with a $1+$ charge.



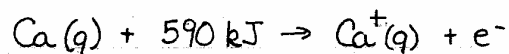
I.E. = 419 kJ/mol of $K(g)$ atoms



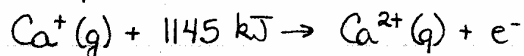
For	$^{39}_{19}K^+$
#p	19
#e	18 (it lost)
#n	20

For calcium:

First ionization energy, IE_1



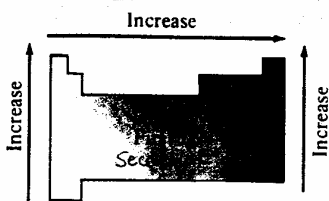
Second ionization energy, IE_2



$IE_2 > IE_1$, since it is more difficult to remove an electron from a positively charged species than a neutral one

Again, IE measures how tightly the electrons are bound to the atom.

As $IE \uparrow$, the difficulty in removing an electron \uparrow



General trend in IE_1 of A Group Elements with position in periodic table. Exceptions occur at IIIA and VIA. These can be explained by quantum mechanics (see pp 226)

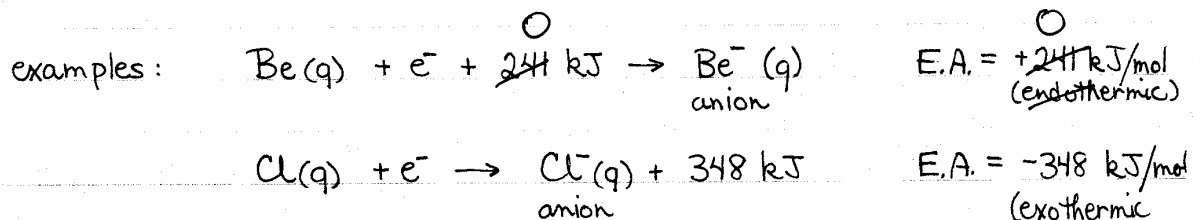
\therefore the outer He electron is more tightly bound than any other (has highest IE_1)

the outer Cs electron is the easiest to remove (has lowest IE_1)

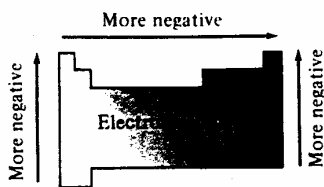
(Note: Fr is ignored because it is rare and radioactive)

Knowledge of the relative values of IE_1 assist in predicting which elements form covalent bonds (by sharing electrons) and which form ionic bonds (electrons are transferred from one atom to another)

(3) Electron Affinity: the amount of energy involved in the process in which an electron is added to an isolated gaseous atom to form an ion with a 1- charge.



for ${}_{17}^{35}\text{Cl}^-$ #p = 17
 #e = 18 (change of -1 means 1 extra electron)
 #n = 18



General trend in electron affinities of A group elements with position in periodic table.
 There are many exceptions.

- ∴ it is easier to add an electron going from left to right or bottom to top.
- ∴ halogens gain electrons easily - have more negative electron affinities.

(4) Ionic Radii

Most parent atoms will react with other atoms in order to gain a noble gas configuration, by either gaining or losing electrons.

LEFT SIDE
OF
PERIODIC
TABLE

Group	IA	IIA	IIIA
electronic config ⁿ	ns ¹	ns ²	ns ² np ¹
electrons lost	1	2	3
final charge on ion	+1	+2	+3

Atoms in these groups will lose electrons to form cations and become positively charged.

In periods 2 and 3, ions from IA, IIA and IIIA are ISOELECTRONIC (have the same total number of electrons).

eg ${}_{11}\text{Na}^+$, ${}_{12}\text{Mg}^{2+}$ and ${}_{13}\text{Al}^{3+}$ all have 10 electrons and are isoelectronic with the noble gas, ${}_{10}\text{Ne}$, neon.

In order of decreasing ionic radii: $\text{Na}^+ > \text{Mg}^{2+} > \text{Al}^{3+}$ since as more electrons are removed, the remaining electrons are held more tightly.

Also, $\text{Na} > \text{Na}^+$, $\text{Mg} > \text{Mg}^{2+}$

RIGHT SIDE
OF
PERIODIC
TABLE

Group	VA	VIA	VIIA
electronic config ⁿ	ns^2np^3	ns^2np^4	ns^2np^5
electrons gained	3	2	1
final charge on ion	-3	-2	-1

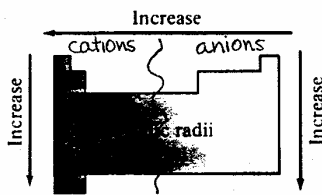
Atoms in these groups will gain electrons to have noble gas configuration - they form anions

Example: In period 2, ${}^7\text{N}^{3-}$, ${}^8\text{O}^{2-}$ and ${}^9\text{F}^-$ all have 10 electrons and are isoelectronic with ${}^{10}\text{Ne}$, ${}^{11}\text{Na}^+$, ${}^{12}\text{Mg}^{2+}$ and ${}^{13}\text{Al}^{3+}$.

In order of decreasing ionic radii $\text{N}^{3-} > \text{O}^{2-} > \text{F}^-$. As electrons are added to a neutral atom, the electron cloud is expanded. Therefore $\text{N}^{3-} > \text{N}$

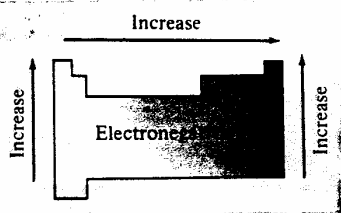
To generalize: eg $\text{H}^- > \text{H} > \text{H}^+$

- (1) simple negatively charged ions (anions) are always larger than parent atom.
- (2) simple positively charged ions (cations) are always smaller than parent atom.
- (3) within an isoelectronic series, atomic radii decrease as atomic no. increases.



General trend in ionic radii of A Group elements with position in periodic table.

(5) Electronegativity: a measure of the relative tendency of an atom to attract electrons to itself when chemically combined with another atom.
(These values appear on the periodic table in the exam)



General trend in electronegativity of A Groups with position in periodic table.

F highest EN (4.0)

O next highest EN (3.5)

Range
0.8 → 4.0
Fr F

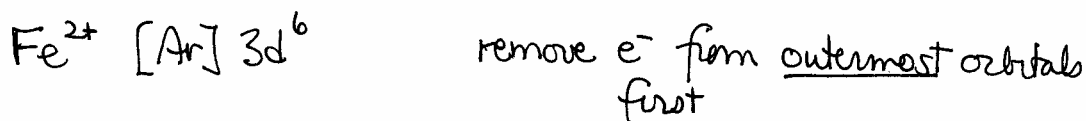
Electronegativity is used to help assign oxidation numbers.

In a simple binary (2 element) compound, the more electronegative element "wants" electrons more and "gets" the negative oxidation number.

Examples:

no.	+1	-1	+1	-1	-3	+1
	Na	Cl	Na	H	N	H ₃
N	1.0	3.0	1.0	2.1	3.0	2.1

Note: Configuration of transition metal ions



So, the order you put e⁻ into orbitals (order of increasing energy) is different from how you remove e⁻ from orbitals.