

**ATOMIC STRUCTURE** (Notes)

**1 Atomic structure**

**1.1 Particles in the atom and atomic radius**

**Learning outcomes**

Candidates should be able to:

- 1 understand that atoms are mostly empty space surrounding a very small, dense nucleus that contains protons and neutrons; electrons are found in shells in the empty space around the nucleus
- 2 identify and describe protons, neutrons and electrons in terms of their relative charges and relative masses
- 3 understand the terms atomic and proton number; mass and nucleon number
- 4 describe the distribution of mass and charge within an atom
- 5 describe the behaviour of beams of protons, neutrons and electrons moving at the same velocity in an electric field
- 6 determine the numbers of protons, neutrons and electrons present in both atoms and ions given atomic or proton number, mass or nucleon number and charge
- 7 state and explain qualitatively the variations in atomic radius and ionic radius across a period and down a group

**1.2 Isotopes**

**Learning outcomes**

Candidates should be able to:

- 1 define the term isotope in terms of numbers of protons and neutrons
- 2 understand the notation  ${}^x_y\text{A}$  for isotopes, where  $x$  is the mass or nucleon number and  $y$  is the atomic or proton number
- 3 state that and explain why isotopes of the same element have the same chemical properties
- 4 state that and explain why isotopes of the same element have different physical properties, limited to mass and density

**1.3 Electrons, energy levels and atomic orbitals**

In 1.3 each atom or ion described will be in the ground state. Only the elements hydrogen to krypton will be assessed.

**Learning outcomes**

Candidates should be able to:

- 1 understand the terms:

- shells, sub-shells and orbitals
  - principal quantum number (n)
  - ground state, limited to electronic configuration
- 2 describe the number of orbitals making up s, p and d sub-shells, and the number of electrons that can fill s, p and d sub-shells
  - 3 describe the order of increasing energy of the sub-shells within the first three shells and the 4s and 4p sub-shells
  - 4 describe the electronic configurations to include the number of electrons in each shell, sub-shell and orbital
  - 5 explain the electronic configurations in terms of energy of the electrons and inter-electron repulsion
  - 6 determine the electronic configuration of atoms and ions given the atomic or proton number and charge, using either of the following conventions:  
e.g. for Fe:  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$  (full electron configuration)  
or [Ar]  $3d^6 4s^2$  (shorthand electron configuration)
  - 7 understand and use the electrons in boxes notation  
e.g. for Fe: [Ar] 

↑↓	↑	↑	↑	↑	↑	↑↓
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  - 8 describe and sketch the shapes of s and p orbitals
  - 9 describe a free radical as a species with one or more unpaired electrons

#### 1.4 Ionisation energy

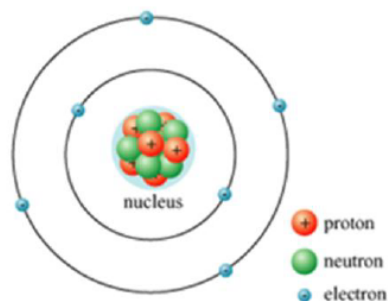
In 1.4 each atom or ion described will be in the ground state. Only the elements hydrogen to krypton will be assessed.

##### Learning outcomes

Candidates should be able to:

- 1 define and use the term first ionisation energy, IE
- 2 construct equations to represent first, second and subsequent ionisation energies
- 3 identify and explain the trends in ionisation energies across a period and down a group of the Periodic Table
- 4 identify and explain the variation in successive ionisation energies of an element
- 5 understand that ionisation energies are due to the attraction between the nucleus and the outer electron
- 6 explain the factors influencing the ionisation energies of elements in terms of nuclear charge, atomic/ionic radius, shielding by inner shells and sub-shells and spin-pair repulsion
- 7 deduce the electronic configurations of elements using successive ionisation energy data
- 8 deduce the position of an element in the Periodic Table using successive ionisation energy data

Introduction to Atom



As you read in O – Level, the whole mass of an atom is concentrated in the central region called nucleus. Protons and neutrons are present in nucleus whereas electrons revolve in orbits.

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Figure shows the atomic structure of oxygen.

Every element is represented by a symbol. These symbols are derived from Latin, Greek or English words.

The sub-atomic particles

Protons, neutrons and electrons.

	relative mass	relative charge
proton	1	+1
neutron	1	0
electron	1/1836	-1

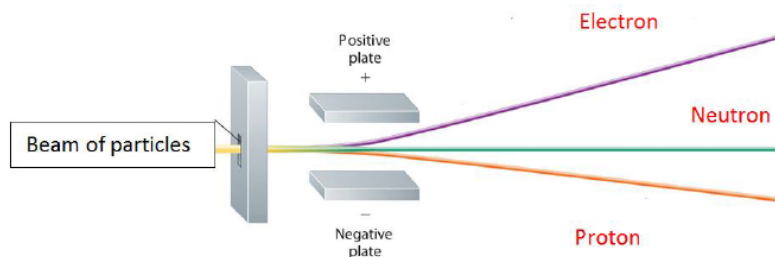
Sub – atomic particles in electric fields

What happens if a beam of each of these particles is passed between two electrically charged plates - one positive and one negative

**Protons** are positively charged and so would be deflected on a curving path towards the negative plate.

**Electrons** are negatively charged and so would be deflected on a curving path towards the positive plate.

**Neutrons** don't have a charge, and so would continue on in a straight line.



Nucleon No

is the sum of protons

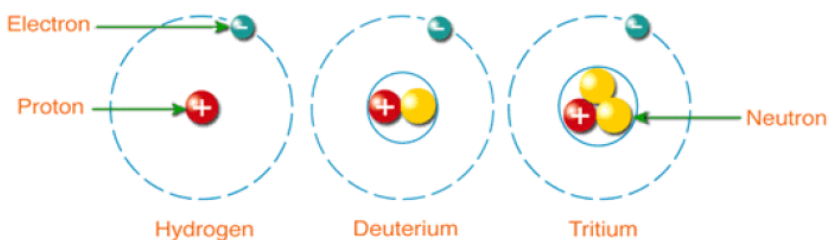
and neutrons present in a nucleus. Complete the following table.

	Protons	Electrons	Neutrons
Sodium ${}^{23}_{11}\text{Na}$			
Calcium ion ${}^{40}_{20}\text{Ca}^{+2}$			
Chlorine ion ${}^{35}_{17}\text{Cl}^{-}$			

**ISOTOPES:-** are the atoms, which have the same atomic number but different mass numbers.

OR.

Isotopes are atoms with same no of protons but different no of neutrons. e.g. Hydrogen has 3 isotopes. Their Structures are shown :



Chlorine-35 and Chlorine -37 are examples of isotopes.  ${}^{35}_{17}\text{Cl}$  and  ${}^{37}_{17}\text{Cl}$

Average mass of isotopes can be calculated if we know their relative abundance. Cl – 35 is 75% and Cl – 37 is 25%.

$$= \frac{35 \times 75 + 37 \times 25}{100} = 35.5$$

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## Electronic Configuration

The principal quantum shells (Orbits) can be divided into subshells. The levels (or shells) are numbered as 1, 2, 3, 4, 5, etc. and the subshells (Orbitals) are indicated by the letters s, p, d, or f.

Principal Quantum Shell	No of Electrons( $2n^2$ )	Orbital
1	2	s
2	8	s, p
3	18	s p d
4	32	s p d f

First principal quantum shell can have maximum 2 electrons. These 2 electrons are present in s orbitals.

2<sup>nd</sup> shell can have maximum 8 electrons. 2 are present in s subshell and 6 are present in p subshell. Similarly in

3<sup>rd</sup> shell, maximum 18 electrons can be present. 2 in s subshell, 6 in p subshell and 10 in d subshell can be present.

NOTE:- s = sharp, p = principal, d= diffuse

### Division of Sub - Shells

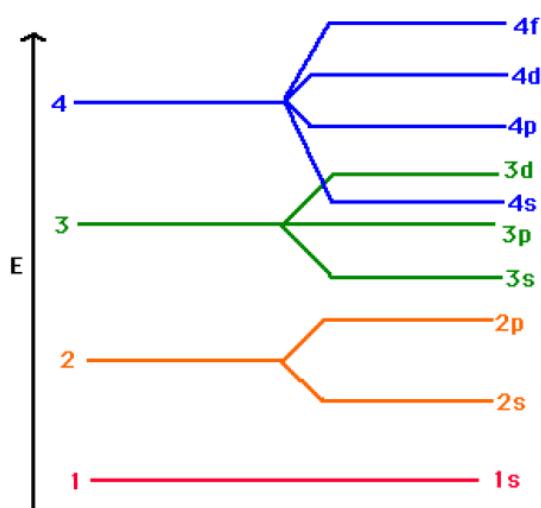
Each orbital can have maximum 2 electrons. The number of orbitals in each subshell must be

Sub Shells	Max Electrons
s	2
p	6
d	10
f	14

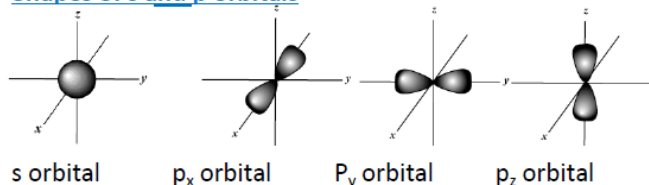
Subshell	Atomic orbitals	Total Electrons
s	s	$1 * 2 = 2$
p	p p p	$3 * 2 = 6$
d	d d d d	$5 * 2 = 10$
f	f f f f f f f f	$7 * 2 = 14$

NOTE:- s has only one orbital  
p orbitals are named as  $p_x$ ,  $p_y$  and  $p_z$ . These orbitals are degenerate. d orbitals are named as  $d_{xy}$ ,  $d_{yz}$ ,  $d_{zx}$ ,  $d_{x^2-y^2}$ ,  $d_{z^2}$ . These orbitals are also degenerate

### Energy level of orbitals



### Shapes of s and p orbitals



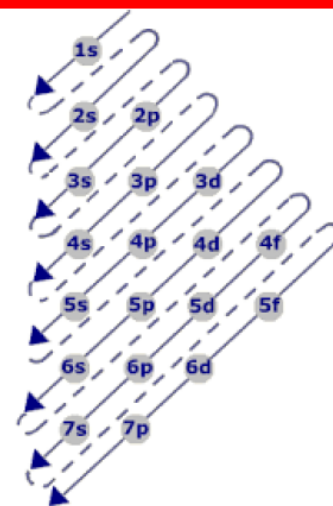
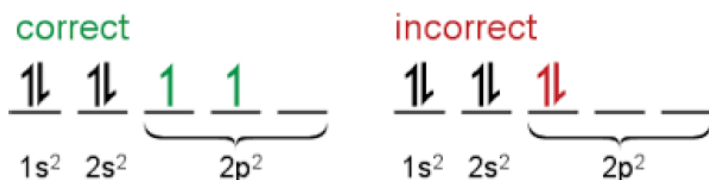
An s orbital has a spherical shape. The 2s orbital has the same shape as the 1s orbital. Electrons of 2s have more energy than the electrons of 1s.

There are three p orbitals. Each p orbital has two lobes as shown in shape. These three orbitals are at right angles to each other so they are named as  $p_x$ ,  $p_y$  and  $p_z$ . These three p orbitals have same energy level.

**Filling orbitals**

Three important rules for filling electrons in orbitals are as

- I. Aufbau Rule. Lowest energy orbitals are filled first. Thus, the filling pattern is 1s, 2s, 2p, 3s, 3p, 4s, 3d, etc.
- II. Hund's Rule. Electrons prefer to live as unpaired electron in orbitals as long as possible, all possessing the same spin direction.
- III. Pauli Exclusion Principle. Only two electrons are permitted per orbital and they must be of opposite spin.



Atomic Number	Element	Electronic configuration	Atomic Number	Element	Electronic configuration
1	H	$1s^1$	9	F	$1s^2 2s^2 2p^5$
2	He	$1s^2$	10	Ne	$1s^2 2s^2 2p^6$
3	Li	$1s^2 2s^1$	11	Na	$1s^2 2s^2 2p^6 3s^1$
4	Be	$1s^2 2s^2$	12	Mg	$1s^2 2s^2 2p^6 3s^2$
5	B	$1s^2 2s^2 2p^1$	13	Al	$1s^2 2s^2 2p^6 3s^2 3p^1$
6	C	$1s^2 2s^2 2p^2$	14	Si	$1s^2 2s^2 2p^6 3s^2 3p^2$
7	N	$1s^2 2s^2 2p^3$	15	P	$1s^2 2s^2 2p^6 3s^2 3p^3$
8	O	$1s^2 2s^2 2p^4$	16	S	$1s^2 2s^2 2p^6 3s^2 3p^4$

**Orbitals in boxes form.**

Orbitals can be represented as boxes. Each box shows one orbital. Electrons are represented as arrows, direction of arrows show spin of electrons. When two electrons are present in orbital, then there arrows are in opposite direction.

			1s	2s	2p <sub>x</sub>	2p <sub>y</sub>	2p <sub>z</sub>
Lithium, Li	$1s^2 2s^1$		$\uparrow\downarrow$	$\uparrow$			
Beryllium, Be	$1s^2 2s^2$		$\uparrow\downarrow$	$\uparrow\downarrow$			
Boron, B	$1s^2 2s^2 2p^1$		$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$		
Carbon, C	$1s^2 2s^2 2p^2$		$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$	$\uparrow$	
Nitrogen, N	$1s^2 2s^2 2p^3$		$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$	$\uparrow$	$\uparrow$
Oxygen, O	$1s^2 2s^2 2p^4$		$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$	
Fluorine, F	$1s^2 2s^2 2p^5$		$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow$
Neon, Ne	$1s^2 2s^2 2p^6$		$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$

NOTE:- electronic configuration of Chromium and copper.

Chromium has  $[\text{Ar}]3d^5 4s^1$  and copper has  $[\text{Ar}] 3d^{10} 4s^1$

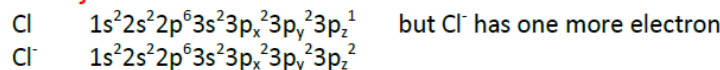
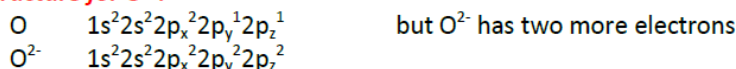
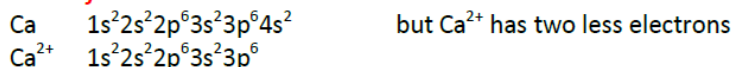
These elements do not follow the pattern.

**Electronic configuration of ions**

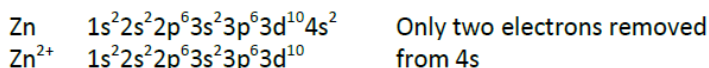
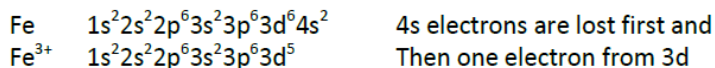
Ions are the atoms or groups of atoms which carry an electric charge because they have either gained or lost one or more electrons. If atom gains electrons it acquires a negative charge. If it loses electrons, it becomes positively charged.

**Electronic structure of s and p block ions.**

Electronic configuration of ion can be written like atom. For -ve ions, electrons are added and for +ve ions, electrons are subtracted.

**To write the electronic structure for Cl<sup>-</sup>:****To write the electronic structure for O<sup>2-</sup>:****To write the electronic structure for Na<sup>+</sup>:****To write the electronic structure for Ca<sup>2+</sup>:****The electronic structure of d-block ions**

Note:- When these metals form ions, the 4s electrons are always lost first.

**To write the electronic structure for Zn<sup>2+</sup>:****To write the electronic structure for Fe<sup>3+</sup>:****Ionization Energy  $\Delta H_i$** 

Ionization energy is the energy required to remove an electron from a gaseous atom or ion.

**1<sup>st</sup> Ionization Energy**

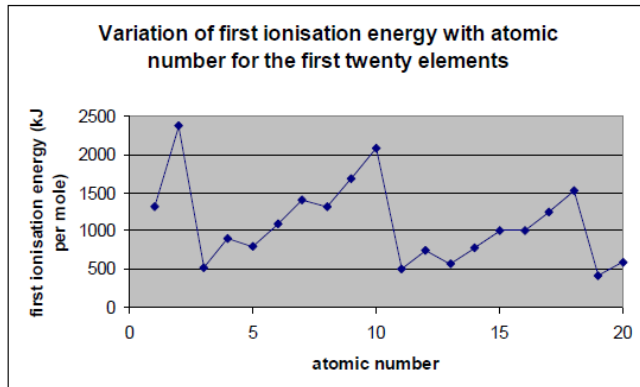
The first ionization energy of an atom is the energy required to remove one mole of electrons from one mole of isolated gaseous atoms to form one mole of 1+ ion.



The first ionization energy of hydrogen can be written as



### Patterns of first ionisation energies in the Periodic Table



First ionisation energy is different for different elements as shown in graph. This graph shows a periodicity. From Li to Ne, it is increasing, then again increasing from Na to Ar.

various trends in this graph which can be explained by reference to the proton number and electronic configuration of the various elements. A number of factors must be considered

#### Factors Affecting the ionization energies

- I. The charge on the nucleus
- II. The distance of the electron from the nucleus.
- III. Shielding Effect
- IV. Electron paired or unpaired

##### 1. The charge on the nucleus

Energy is required to remove electrons from atoms in order to overcome their attraction to the nucleus. The greater the number of protons, the greater the attraction of the electrons to the nucleus and the harder it is to remove the electrons. The number of protons in the nucleus is known as the **nuclear charge**

##### 2. The distance of the electron from the nucleus

Attraction falls off very rapidly with distance. An electron close to the nucleus will be much more strongly attracted than one further away

##### 3. Shielding Effect

The effect of nuclear charge, however, is cancelled out to some extent by the other electrons in the atom. Each inner shell and inner sub-shell electron effectively cancels out one unit of charge from the nucleus. This is known as **shielding**

##### 4. Electron paired or unpaired

Two electrons in the same orbital experience a bit of repulsion from each other. This offsets the attraction of the nucleus, so that paired electrons are removed rather more easily than you might expect.

#### Explaining I.E of first few elements

**Hydrogen** has an electronic structure of  $1s^1$ . It is a very small atom, and the single electron is close to the nucleus and therefore strongly attracted. There are no electrons screening it from the nucleus and so the ionisation energy is high ( $1310 \text{ kJ mol}^{-1}$ ).

**Helium** has a structure  $1s^2$ . The electron is being removed from the same orbital as in hydrogen's case. It is close to the nucleus and unscreened. The value of the ionisation energy ( $2370 \text{ kJ mol}^{-1}$ ) is much higher than hydrogen, because the nucleus now has 2 protons attracting the electrons instead of 1.

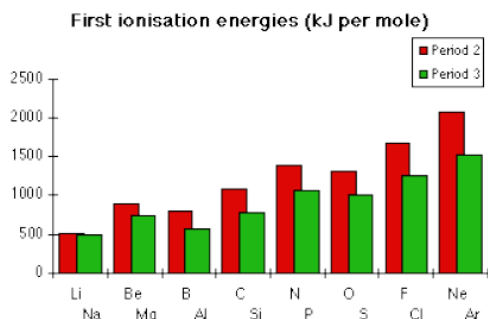
**Lithium** is  $1s^2 2s^1$ . Its outer electron is in the second energy level, much more distant from the nucleus. You might argue that that would be offset by the additional proton in the nucleus, but the electron doesn't feel the full pull of the nucleus - it is screened by the  $1s^2$  electrons but the distance is important so Lithium's first ionisation energy drops to  $519 \text{ kJ mol}^{-1}$ , whereas hydrogen's is  $1310 \text{ kJ mol}^{-1}$ .

H	1312	N	1402
He	2372	O	1314
Li	520	F	1680
Be	899	Ne	2080
B	800	Na	496
C	1086	Mg	737

## Trends in Ionization Energy

### Trends across period

In general, the first ionisation energy increases across a period because the nuclear charge increases but the shielding remains the same.



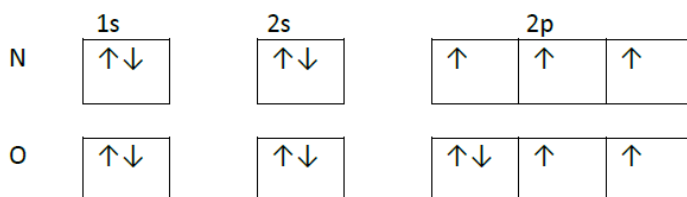
Compare the first ionisation energies of Li ( $1s^2 2s^1$ ) and Be ( $1s^2 2s^2$ ). Be has one more proton in the nucleus than Li, and no extra inner-shell electrons, so the effective nuclear charge on Be is higher and the Be electrons are more strongly attracted to the nucleus. Thus the first ionisation energy of Be is higher than that of Li.

Compare the first ionisation energies of Be ( $1s^2 2s^2$ ) and B ( $1s^2 2s^2 2p^1$ ). B has one more proton in the nucleus than Be but there are also 2 extra inner sub-shell electrons. So 2p1 electron of B has more shielding than Be. So B electrons are less strongly attracted to the nucleus and

thus less difficult to remove. Thus the first ionisation energy of B is lower than that of Be.

From B ( $1s^2 2s^2 2p^1$ ) to N ( $1s^2 2s^2 2p^3$ ) the proton number increases, but the number of electrons shielding the nuclear charge remains the same. Thus the effective nuclear charge increases from B to N and the electrons become progressively harder to remove and Thus the first ionisation energy increases from B to N.

The electronic configurations of N and O must be considered more carefully:



Note that in N the electron is removed from an unpaired orbital, but in O it is removed from a paired orbital. In a paired orbital, the two electrons share a confined space and so repel each other. They are therefore less stable and easier to remove. This repulsion effect reduces the higher effective nuclear charge in O.

Thus the first ionisation energy of O is lower than that of N. The first ionisation energies increase as expected from O to Ne, due to the increase in effective nuclear charge.

So in period 2 the first ionisation energy increases across a period but two exceptions are seen,

- I. the first ionisation energy of B is lower than that of Be
- II. the first ionisation energy of O is lower than that of N

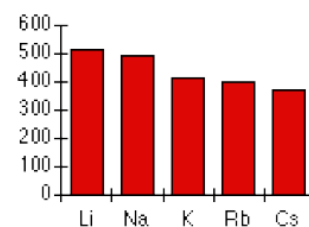
The same trend can also be found in Period 3 (Na - Ar). There is a general increase, but a drop between Mg and Al and also between P and S.

### Trend down a group

As you go down a group in the Periodic Table ionisation energies generally fall.

This is because the electron to be removed from the outer energy level is increasingly distant from the nucleus, as a result the attraction of the nucleus for the electron becomes less, and it becomes easier to pull electron away.

First ionisation energies (kJ per mole)





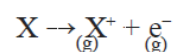
Electrons in the inner energy levels also produce a screening effect. These inner electrons reduce the attraction of the nucleus for the outer electrons. The screening effect will increase as the number of inner energy levels increases.

### Successive Ionization Energy

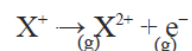
The amount of energy needed for removing all the electrons (one by one) of a gaseous atom is known as successive ionization energies. These are basically termed as 1st, 2nd, 3rd or 4th ..... ionization energy and these depends completely on the removal of the 1st, 2nd, 3rd electrons respectively.

- 2<sup>nd</sup> ionization Energy: It is the energy needed to remove a second electron from each ion in 1 mole of gaseous 1+ ions to give gaseous 2+ ions.
- 3<sup>rd</sup> ionization Energy: It is the energy needed to remove a third electron from each ion in 1 mole of gaseous 2+ ions to give gaseous 3+ ions.

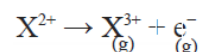
1st ionization energy



2nd ionization energy



3rd ionization energy



### Finding electronic configuration of an element

Once you have removed the first electron you are left with a positive ion. Trying to remove a negative electron from a positive ion is going to be more difficult than removing it from an atom. Removing an electron from a 2+ or 3+ (etc) ion is going to be progressively more difficult. So the value of successive ionization energies increase. This increase in values are very helpful in finding the electronic structure of atoms.

Table Shows the Successive ionization Energies of first 13 elements

	Proton number	First	Second	Third	Fourth
H	1	1310	–	–	–
He	2	2370	5250	–	–
Li	3	519	7300	11800	–
Be	4	900	1760	14800	21000
B	5	799	2420	3660	25000
C	6	1090	2350	4610	6220
N	7	1400	2860	4590	7480
O	8	1310	3390	5320	7450
F	9	1680	3370	6040	8410
Ne	10	2080	3950	6150	9290
Na	11	494	4560	6940	9540
Mg	12	736	1450	7740	10500
Al	13	577	1820	2740	11600

#### Example:- Electronic Structure of Lithium from I.E

The successive ionization energies of Lithium are as

519	7300	11800
2s	1s	1s

This shows that there are three electrons, 1 in the outermost sub – shell and two in inner sub – shell. So the inner sub shell is 1s and Outer sub shell is 2s. The electronic configuration will be as 1s<sup>2</sup>, 2s<sup>1</sup>.

This configuration also shows that there are two principal quantum shell as there is a big jump (multiples of 519) in values from 519 to 7300.



