



唯寻国际教育

橡泳国际教育

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Lecture 1 The period trends and molecular structures

Test situation analysis

| Testing points | Occurrence (2010-2021) |
|---|------------------------|
| Atomic structure and Isotopes | 5 |
| Electron configuration | 5 |
| Period table trend | 2 |
| Bonding and dot-cross | 13 |
| VSEPR and Determination of the molecular geometry | 7.5 |
| Intermolecular forces and boiling point | 2 |

Intensive Teaching and Practicing

Point 1: Atom structure

1.1. Atom structure

The atom contains two parts, central, positively charged nucleus and negatively charged electrons which orbit around the central nucleus.

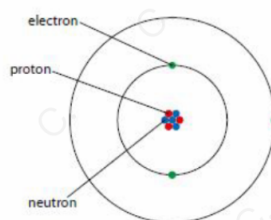
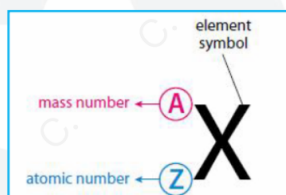


Figure 1.1 A simple representation of a lithium atom (not to scale)

All the mass of the atom is concentrated in the nucleus.

1.2 Isotopes



(Figure 1.2 Chemistry for IB Diploma Cambridge textbook p57)

- ✓ The atomic number (Z) is the number of protons in the nucleus.
- ✓ The mass number or nucleon number is the number of protons plus neutrons in the nucleus
- ✓ **number of neutrons = mass number - number of proton**
- ✓ For an atom, **number of electron = number of proton**, because the overall charge on an atom is zero.

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Definition: isotopes are atoms of the same element which have the same number of protons, but different number of neutrons.

For example: ${}^1_1\text{H}$ ${}^2_1\text{H}$ ${}^3_1\text{H}$

Isotopes property:

Isotopes have the same chemical properties (they react in the same way) but different physical properties (for example, melting point or boiling point).

Isotopes have the same chemical properties because they have the same number of electrons and electronic configuration.

isotopic masses, we can calculate the relative atomic mass of the element very accurately.

To find the necessary data we use an instrument called a mass spectrometer .The mass spectrum produced shows the relative abundance (isotopic abundance) on the vertical axis and the mass to ion charge ratio (m/e) on the horizontal axis. Figure 1.3 shows a typical mass spectrum for a sample of neon.

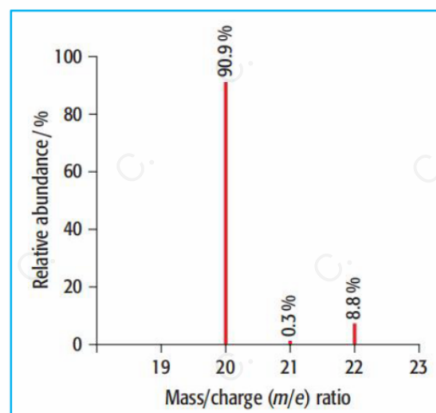


Fig 1.3 — 《Cambridge International AS and A Level Chemistry Coursebook 》 P4

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The mass spectrum of neon has three peaks:

^{20}Ne (90.9%), ^{21}Ne (0.3%) and ^{22}Ne (8.8%).

$$A_r \text{ of neon} = \frac{(20 \times 90.9) + (21.0 \times 0.3) + (22 \times 8.8)}{100} = 20.2$$

Example 1.(source. UKChO.2018.3b-3c)

The accurate relative atomic mass of uranium found in the Earth's crust is 238.0289. The accurate relative atomic mass of the ^{238}U isotope is 238.0507.

^{235}U (accurate relative atomic mass = 235.0439)

(b) Assuming only ^{235}U and ^{238}U are present, calculate the percentage abundance in the Earth's crust of:

(i) ^{235}U

(ii) ^{238}U

For use in nuclear weapons, a sample of uranium must contain at least 80% of the ^{235}U isotope. As this is a much higher percentage of ^{235}U than found in the crust, the amount of ^{235}U must be enriched artificially. The enrichment of the ^{235}U isotope is performed by converting the uranium to uranium hexafluoride (UF_6), which is a gas above 57 °C. The two different isotopic forms of uranium hexafluoride gas ($^{235}\text{UF}_6$ and $^{238}\text{UF}_6$) can be separated in a centrifuge.

(c) Which property of fluorine is essential for the successful separation of $^{235}\text{UF}_6$ and $^{238}\text{UF}_6$ in a gas centrifuge? Circle the correct answer in the answer booklet.

- A. Elemental fluorine exists as diatomic molecules.
- B. Fluorine has only one naturally occurring isotope.
- C. Fluorine has the highest electronegativity of all elements.
- D. Fluorine is a gas at room temperature and pressure.
- E. Fluorine reacts vigorously with most metals.



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Exercise 1. (source. UKChO. 2019.2)

The gold and platinum react with the aqua regia to form solutions of chloroauric acid (HAuCl_4) and chloroplatinic acid (H_2PtCl_6), as well as nitrogen dioxide.

Mass spectrometry can be used to identify the chloroauric acid. Naturally occurring chlorine exists as two isotopes ^{35}Cl (75% abundance) and ^{37}Cl (25% abundance). ^{197}Au is 100% abundant.

(c) Calculate the m/z values and intensities of the molecular ion peaks for the AuCl_4^- ion as a percentage of the total. Use integer masses in the calculation.





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Point 2: Electron configuration

2.1 the principle quantum number: n

The orbits with the same main quantum number are divided into an electronic layer, and the electronic layer symbols K, L, M, N, O and P correspond to $n = 1, 2, 3, 4, 5, 6$, etc. The greater n , the greater the average distance from the nucleus.

The number of electrons that each electron layer can hold can be calculated as $2n^2$. (This rule applies only if n is less than or equal to 4)

The lowest energy level, $n = 1$, is closest to the nucleus, the energy level $n = 2$ is further out, and so on.

Each principal quantum shell can hold a maximum number of electrons:

$n=1$ shell 1 – up to 2 electrons

$n=2$ shell 2 – up to 8 electrons

$n=3$ shell 3 – up to 18 electrons

$n=4$ shell 4 – up to 32 electrons.

2.2 the azimuthal quantum number (l)

In chemistry, the angular momentum quantum number is a quantum number that describes the 'shape' of an orbital and tells us which subshells are present in the principal shell. The symbol that is used when we refer to the angular momentum quantum number is " l ".

| | |
|---------|------------|
| $l = 0$ | s orbital |
| $l = 1$ | p orbitals |
| $l = 2$ | d orbitals |
| $l = 3$ | f orbitals |

2.3 atomic orbitals

Each subshell contains one or more orbitals, **an orbital is a region where there is high possibility of finding an electron, and each orbital can hold up to 2 electrons**, the number of orbitals in each subshell must be:

| | |
|------------|------------|
| s subshell | 1 orbital |
| p subshell | 3 orbitals |
| d subshell | 5 orbitals |
| f subshell | 7 orbitals |

The orbital with angular quantum number l contains $2l + 1$ orbitals.

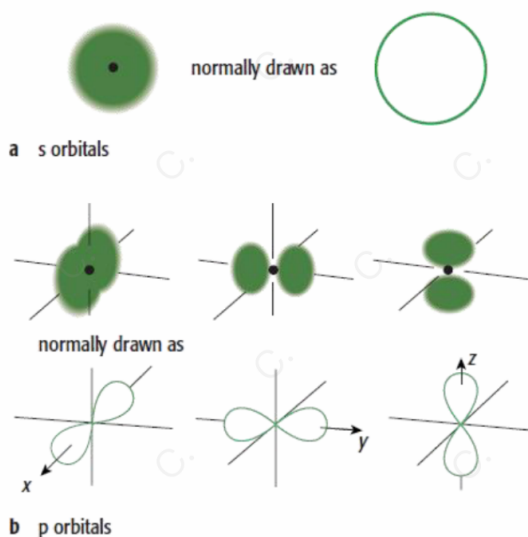
HINT:

the difference between orbitals and subshells:

each p orbital can hold up to 2 electrons, but p subshell which contain 3p orbitals can hold up to 6 electrons in total.

2.4 Shapes of s and p orbitals

Each orbital has a three-dimensional shape. Within this shape there is a high probability of finding the electron or electrons in the orbital.





(Figure 2.1 Cambridge International AS and A Level Chemistry textbook p39)

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The d orbitals are more complex in shape and arrangement in space.

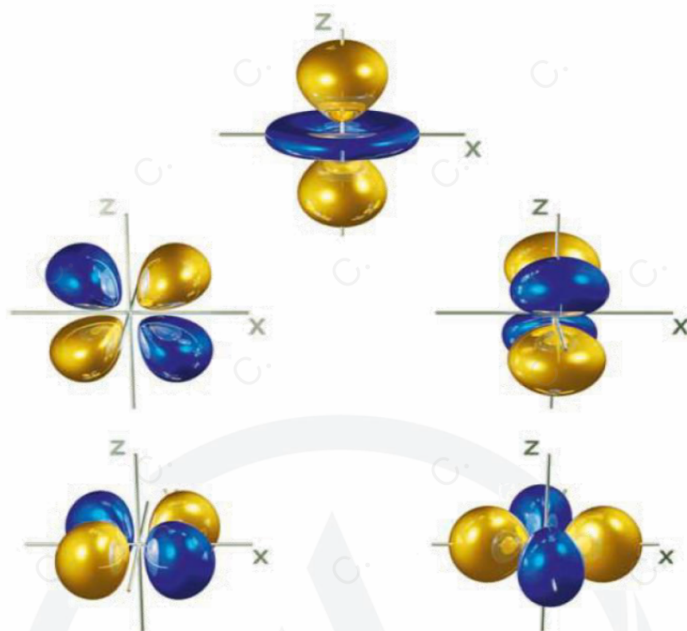
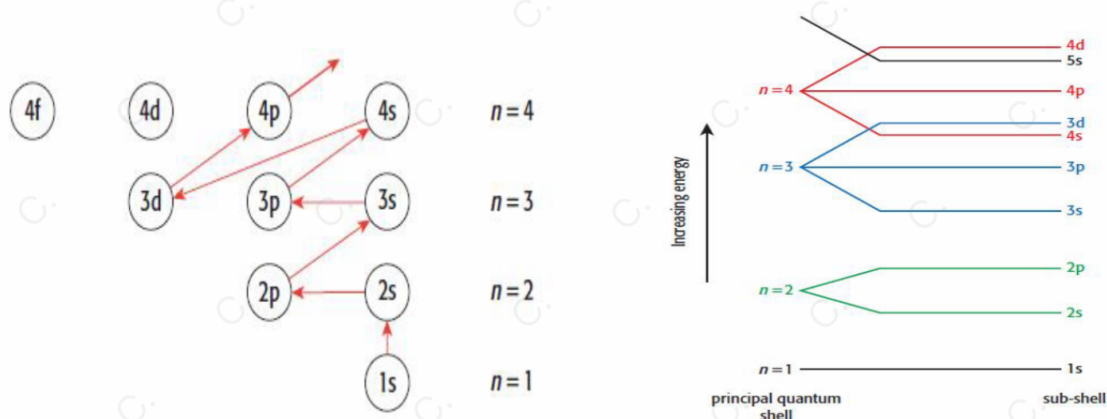


Figure 2.2

2.5 Filling the shells and orbitals

2.5.1 The Aufbau (“building-up”) principle:

The Aufbau (“building-up”) principle, which states that electrons will fill orbitals of lowest energy first. Unfortunately, this order is not a linear sequence from 1 to 7.



(Figure 2.3 Cambridge International AS and A Level Chemistry textbook p37-38)

2.5.2 presenting configurations

A detailed way of writing the electronic configuration of an atom that includes information about the number of electrons in each subshell is shown below for hydrogen.

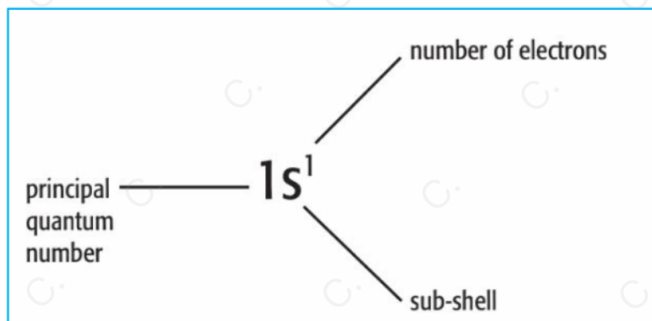


Table 1.1 **The electronic configuration** for elements to 36
(full /condensed electronic configuration)

| Proton number | Symbol | Electronic configuration |
|---------------|--------|----------------------------|
| 1 | H | $1s^1$ |
| 2 | He | $1s^2$ |
| 3 | Li | $1s^2 2s^1$ |
| 4 | Be | $1s^2 2s^2$ |
| 5 | B | $1s^2 2s^2 2p^1$ |
| 6 | C | $1s^2 2s^2 2p^2$ |
| 7 | N | $1s^2 2s^2 2p^3$ |
| 8 | O | $1s^2 2s^2 2p^4$ |
| 9 | F | $1s^2 2s^2 2p^5$ |
| 10 | Ne | $1s^2 2s^2 2p^6$ |
| 11 | Na | $1s^2 2s^2 2p^6 3s^1$ |
| 12 | Mg | $1s^2 2s^2 2p^6 3s^2$ |
| 13 | Al | $1s^2 2s^2 2p^6 3s^2 3p^1$ |
| 14 | Si | $1s^2 2s^2 2p^6 3s^2 3p^2$ |
| 15 | P | $1s^2 2s^2 2p^6 3s^2 3p^3$ |
| 16 | S | $1s^2 2s^2 2p^6 3s^2 3p^4$ |
| 17 | Cl | $1s^2 2s^2 2p^6 3s^2 3p^5$ |
| 18 | Ar | $1s^2 2s^2 2p^6 3s^2 3p^6$ |

| Proton number | Name (Symbol) | Electronic configuration |
|---------------|----------------|---------------------------------|
| 19 | potassium (K) | $[\text{Ar}] 4s^1$ |
| 20 | calcium (Ca) | $[\text{Ar}] 4s^2$ |
| 21 | scandium (Sc) | $[\text{Ar}] 3d^1 4s^2$ |
| 24 | chromium (Cr) | $[\text{Ar}] 3d^5 4s^1$ |
| 25 | manganese (Mn) | $[\text{Ar}] 3d^5 4s^2$ |
| 29 | copper (Cu) | $[\text{Ar}] 3d^{10} 4s^1$ |
| 30 | zinc (Zn) | $[\text{Ar}] 3d^{10} 4s^2$ |
| 31 | gallium (Ga) | $[\text{Ar}] 3d^{10} 4s^2 4p^1$ |
| 35 | bromine (Br) | $[\text{Ar}] 3d^{10} 4s^2 4p^5$ |
| 36 | krypton (Kr) | $[\text{Ar}] 3d^{10} 4s^2 4p^6$ |

When writing some of the lower table configurations the total configuration can be fairly long. In these cases, you can use the previous noble gas to abbreviate the configuration as shown below.

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Ex: Lead

- $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^2$
- $[\text{Xe}] 6s^2 4f^{14} 5d^{10} 6p^2$

【Answer】

Example 1. Use two different way to write the electron configuration of these particles:

S^{2-} Mg

S^{2-} : $1s^2 2s^2 2p^6 3s^2 3p^6$ $[\text{Ne}] 3s^2 3p^6$

Mg : $1s^2 2s^2 2p^6 3s^2$ $[\text{Ne}] 3s^2$

The electron configurations for Cations are also made based on the number of electrons but there is a slight difference in the way they are configured. First you should write their normal electron configuration and then when you remove electrons you have to take them from the outermost shell.

For example:

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

Fe^{3+} $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$

Since 4s is in the outer shell, so we should give priority to losing 4s electrons, the other example is Cu^{2+}

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

Cu^{2+} $1s^2 2s^2 2p^6 3s^2 3p^6 3d^9$

【Answer】

F^- : $1s^2 2s^2 2p^6$

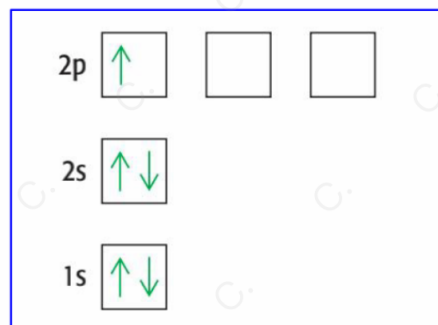
Ti^{2+} : $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2$

Cr^{3+} : $1s^2 2s^2 2p^6 3s^2 3p^6 3d^3$



2.5.3 Orbital diagrams

A useful way of representing electronic configurations is a diagram that places electrons in boxes



- Each box represents an atomic orbital.
- The boxes (orbital) can be arranged in order of increasing energy from bottom to top.
- An electron is represented by an arrow.
- The direction of the arrow represents the 'spin' of the electron. (We imagine an electron rotating around its own axis either in a clockwise or anticlockwise direction.)

⇒ Rules used for putting electron in boxes

The Pauli exclusion principle

- When there are two electrons in an orbital, the 'spins' of the electrons are opposite, so the two arrows in this box point in opposite directions



(Figure 2.4 Chemistry for IB Diploma Cambridge textbook p70)

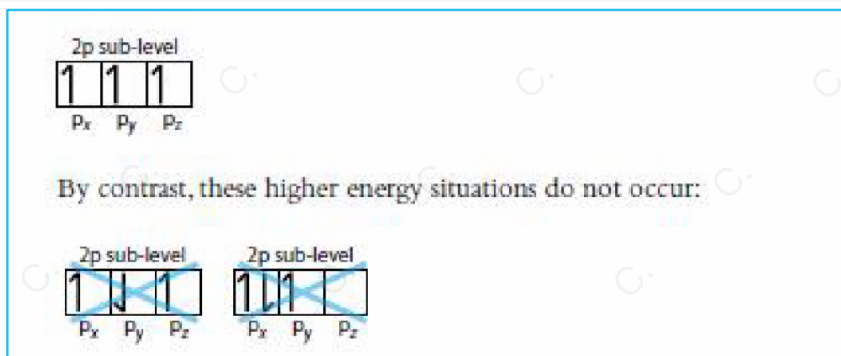
Hund's rule

Hund's rule states that:

1. Every orbital in a sublevel is singly occupied before any orbital is doubly occupied.
2. All of the electrons in singly occupied orbitals have the same spin (to maximize total spin).



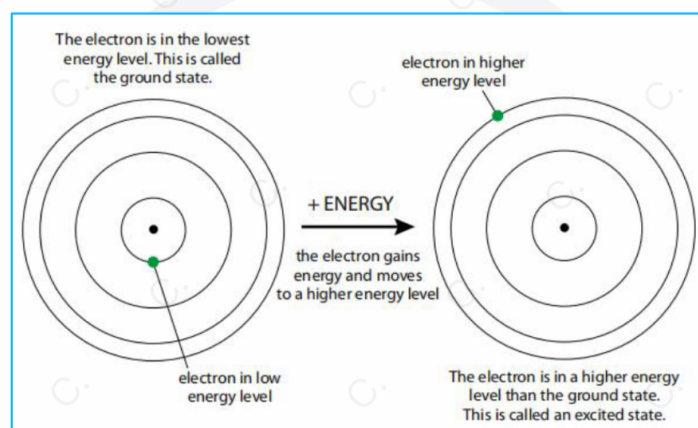
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(Figure 2.5 Chemistry for IB Diploma Cambridge textbook p71)

Supplement:

- 1.Orbital contains only one electron - unpaired electrons.
- 2.Ground state and excited state



(Figure 2.6 IB Chemistry for 2nd editon p64)

Example 2. Which element would have its highest energy valence electron correspond to the following quantum numbers? $n=4, l=2$ (Source: 2016, CCC, a, 8)

- A)Sc B)Y C) K D) Zn E) Ga

Exercise 2. (Source: 2017, CCC, a, 12)

The electron configuration $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$ corresponds to which of the following ?

- A) Ni B) Ni^{2+} C) Fe D) Fe^{2+} E) Zn^{2+}

Exercise 3. (source, UKChO, 2019, 3a)

(a) Identify which element is responsible for each of the electronic structures:

- (i) $[Kr] 4d^{10}$
(ii) $[Xe] 4f^{14} 5d^9 6s^1$
(iii) $[Xe] 4f^{14} 5d^7 6s^2$

2.5.4 The relationship between electron configurations and the periodic table

A careful inspection of the periodic table and Figure 2.7 will allow us to see some very clear relationships between the elements and their electron configurations. Note the configurations for H, Li, Na, and K (all group 1A elements). For each element, the last part of the electron configuration shows s^1 , representing a single electron in the outer s orbital. The other groups of elements show similar patterns. The patterns help us to better understand certain properties of atoms that you will review in the next section. The periodic table is arranged according to the chart shown below:

When writing the electron configurations for an atom, there are a couple of short cut techniques that can be used to help you remember the order in which the orbitals will fill up. The first is the chart in Figure 2.7.

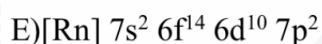
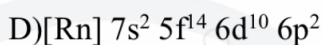
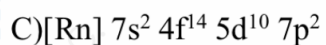
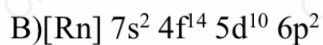
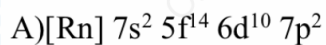


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According to the Aufbau Principle in quantum mechanics, the electrons are arranged according to the energy levels of high and low energy levels, and the general order is as follows: $1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 5f < 6d \dots$
 $< ns < (n-3)g < (n-2)f < (n-1)d < np.$

Example 3.(Source: 2013, CCC, a, 2)

In May 2012, the International Union of Pure and Applied Chemistry (IUPAC) officially approved the names flerovium and livermorium for elements 114 and 116 respectively. The electron configuration of flerovium element 114 is _____



Point 3: Period table trend

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3.1 The periodic table

The periodic table can be classified as **metal**, **non-metal** and **metalloids(also called semi-metal)**.

Metals are shaded yellow in the above periodic table.

(Gp1=alkali metal; Gp2=alkaline earth metal)

Non-metals are shaded pink in the above periodic table.

Metalloids, which have some of properties of both metals and non-metals, are shaded green in the following periodic table.

| group number: | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
|---------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 1 | H 1 | | | | | | | | | | | | | | | | | He 2 |
| 2 | Li 3 | Be 4 | | | | | | | | | | | B 5 | C 6 | N 7 | O 8 | F 9 | Ne 10 |
| 3 | Na 11 | Mg 12 | | | | | | | | | | | Al 13 | Si 14 | P 15 | S 16 | Cl 17 | Ar 18 |
| 4 | K 19 | Ca 20 | Sc 21 | Ti 22 | V 23 | Cr 24 | Mn 25 | Fe 26 | Co 27 | Ni 28 | Cu 29 | Zn 30 | Ga 31 | Ge 32 | As 33 | Se 34 | Br 35 | Kr 36 |
| 5 | Rb 37 | Sr 38 | Y 39 | Zr 40 | Nb 41 | Mo 42 | Tc 43 | Ru 44 | Rh 45 | Pd 46 | Ag 47 | Cd 48 | In 49 | Sn 50 | Sb 51 | Te 52 | I 53 | Xe 54 |
| 6 | Cs 55 | Ba 56 | La 57 | Hf 72 | Ta 73 | W 74 | Re 75 | Os 76 | Ir 77 | Pt 78 | Au 79 | Hg 80 | Tl 81 | Pb 82 | Bi 83 | Po 84 | At 85 | Rn 86 |
| 7 | Fr 87 | Ra 88 | Ac 89 | | | | | | | | | | | | | | | |

(Figure 3.1 page 85 chemistry for IB Diploma coursebook 2nd editions)

The periodic table is divided into blocks according to the highest energy subshell occupied by electrons. So, in the **s** block all the elements have atoms in which the outer shell electron configuration is ns^1 or ns^2 (where n is the shell number).

| period number: gives number of highest main energy level occupied | 1 | 2 | number of electrons in d sub-level | | | | | | | | | | number of electrons in p sub-level | | | | | |
|---|----|----|------------------------------------|----|----|----|----|----|----|----|----|----|------------------------------------|----|----|----|----|----|
| | 1 | 2 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | H | | | | | | | | | | | | | | | | | He |
| 2 | Li | Be | | | | | | | | | | | B | C | N | O | F | Ne |
| 3 | Na | Mg | | | | | | | | | | | Al | Si | P | S | Cl | Ar |
| 4 | K | Ca | Sc | Ti | V | Cr | Mn | Fe | Co | Ni | Cu | Zn | Ga | Ge | As | Se | Br | Kr |
| 5 | Rb | Sr | Y | Zr | Nb | Mo | Tc | Ru | Rh | Pd | Ag | Cd | In | Sn | Sb | Te | I | Xe |
| 6 | Cs | Ba | La | Hf | Ta | W | Re | Os | Ir | Pt | Au | Hg | Tl | Pb | Bi | Po | At | Rn |

← number of electrons in outer shell (groups 1-10)
 ← group number - 10 = number of electrons in outer shell (groups 11-18)
 → 1s²
 → 2s²
 → 3s²
 → 4s²
 → 3d¹⁰
 → 2p⁶
 → 3p⁶
 → 4p⁶

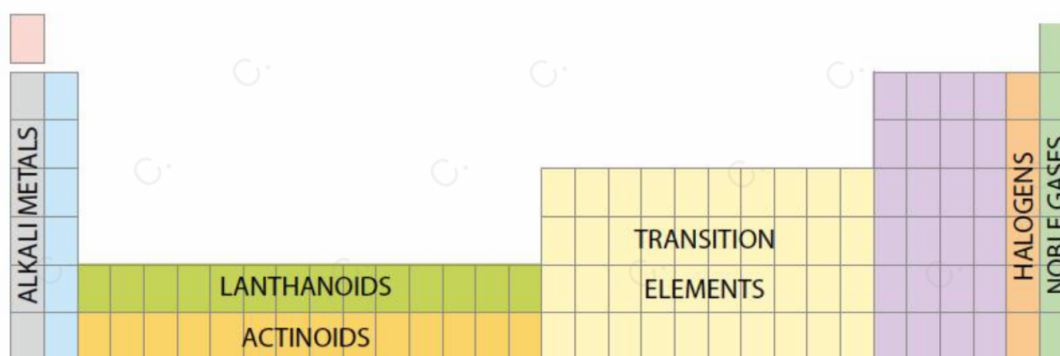
s block d block p block



(Figure 3.2 page 86 chemistry for IB Diploma coursebook 2nd editions)

According to the group number, the periodic table also can be classified as **alkali metals, halogens and noble gases**.

According to the orbital blocks, the periodic table can be classified as **lanthanides, actinides, and transition metals**. Lanthanides and actinides belong to **f** block. Transition metals belong to **d** block.



(Figure 3.3 page 86 chemistry for IB Diploma coursebook 2nd editions)

3.2 Factors affecting the Behavior and Structure of atoms

There are two factors that are closely associated with the structure and behavior of atoms.

⇒ **Nuclear charge**: The nuclear charge is related to the number of charged particles (protons) in the nucleus. As the nuclear charge increases, there is an increase in the attractive force between the nucleus and the electrons. Nuclear charge increases from left to right across a period.

⇒ **Shielding effect**: The shielding effect occurs when electrons in a lower energy level “shield” the electrons in a higher energy level from the effective charge of the nucleus. As a result, the attractive force felt by those outer electrons is less than it would be had those inner electrons not been present. As more energy levels fill, more shielding is seen between the nucleus and the outermost electrons in an atom. Therefore, shielding effect increases, going from top to bottom in a group. Increases in shielding effect are seen only after an energy level is filled and electrons begin to

fill in a further energy level. Therefore, shielding effect does not change going from left to right across a period.

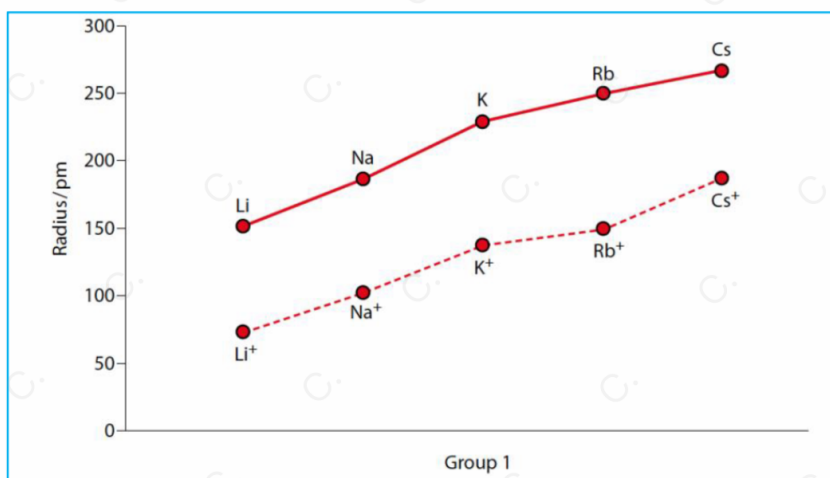
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3.3 Trends in atomic radius

In the same period, the atomic radius decreases from left to right
In the same family, the atomic radius increases from top to bottom

3.3.2 Ionic radius:

The ionic radii of positive ions are smaller than their atomic radii



(Figure 3.4 page 89 chemistry for IB Diploma coursebook 2nd editions)

The ionic radii of negative ions are greater than their atomic radii

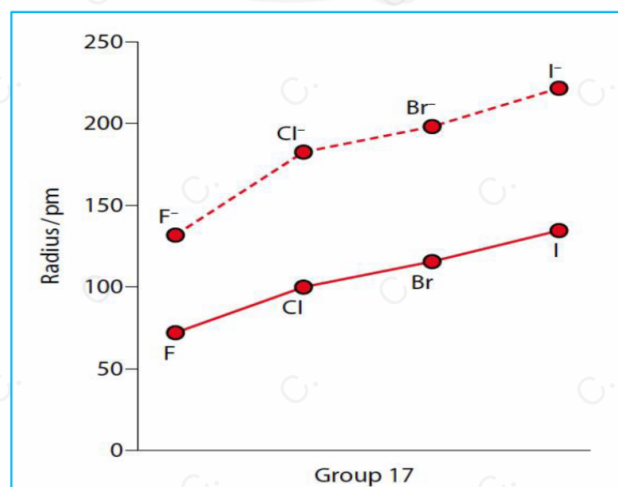


Figure 3.5



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All cations get smaller going across a period and larger going down a group.

For example: $r(\text{Na}^+) > r(\text{Mg}^{2+}) > r(\text{Al}^{3+})$, $r(\text{K}^+) > r(\text{Na}^+) > r(\text{Li}^+)$.

$r(\text{N}^{3-}) > r(\text{O}^{2-}) > r(\text{F}^-)$, $r(\text{F}^-) < r(\text{Cl}^-) < r(\text{Br}^-)$

To compare atomic or ionic radii:

1. First compare the number of electron layers. The more layers, the greater the radius
2. When the number of layers is the same, the larger the atomic number is, the smaller the radius is

Example 4: Arrange the following atoms in order of increasing atomic radius: S, P, O

Exercise 4. (Source: 2018, CCC, a, 20)

Which of the following accurately represents a trend in atomic radius?

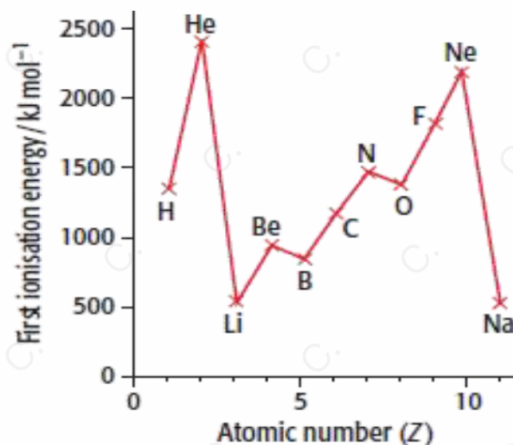
- A) $\text{F} > \text{Cl} > \text{Br}$ B) $\text{F} > \text{O} > \text{N}$ C) $\text{Cl}^- > \text{Na}^+ > \text{Mg}^{2+}$
 D) $\text{Ca}^{2+} > \text{K}^+ > \text{Ca}$ E) $\text{O}^{2-} > \text{S}^{2-} > \text{Cl}$

3.3.3 Ionization energy and successive ionization energies

Ionization energy is the amount of energy necessary to remove an electron from a gaseous atom.

The first ionisation energy: amount of energy required to remove one mol electrons from one mol gaseous atoms.

The general trend is that first ionization energy increases from left to right across a period.



(Figure 3.6 Cambridge International AS and A Level Chemistry textbook p41)

a. First ionization energy increases across the period

b. Ionization energy decrease down the group

c. Group 2 > Group 13

The group 13 elements have the electron configuration ns^2np^1 .

The group 2 elements have the electron configuration ns^2 .

The p orbital has higher energy than s orbitals, which requires less energy to remove outer electron.

d. Group 15 > Group 16

The group 15 elements have the electron configuration ns^2np^3 .

The group 16 elements have the electron configuration ns^2np^4 .

The electron is half-filled in p orbitals of group 15 element, which is stable.

The electrons are paired in the p orbital of group 16 element, the repulsion between electrons reduce the ionization energy, which requires less energy to remove the outer electron.

Exercise:

1. Why the first ionization energy of magnesium is higher than that of sodium.

Magnesium has greater number of protons, and it is smaller than sodium. There is greater attraction between Mg nucleus and electrons.

2. Be and B in period 2

Be $1s^2 2s^2$ and B $1s^2 2s^2 2p^1$. In B, electron is in 2p orbital, which is more shielded. In addition, the 2p sub-level in B is higher in energy than the 2s sub-level in beryllium, and therefore less energy is required to remove an electron from boron.

3. O and N in period 2

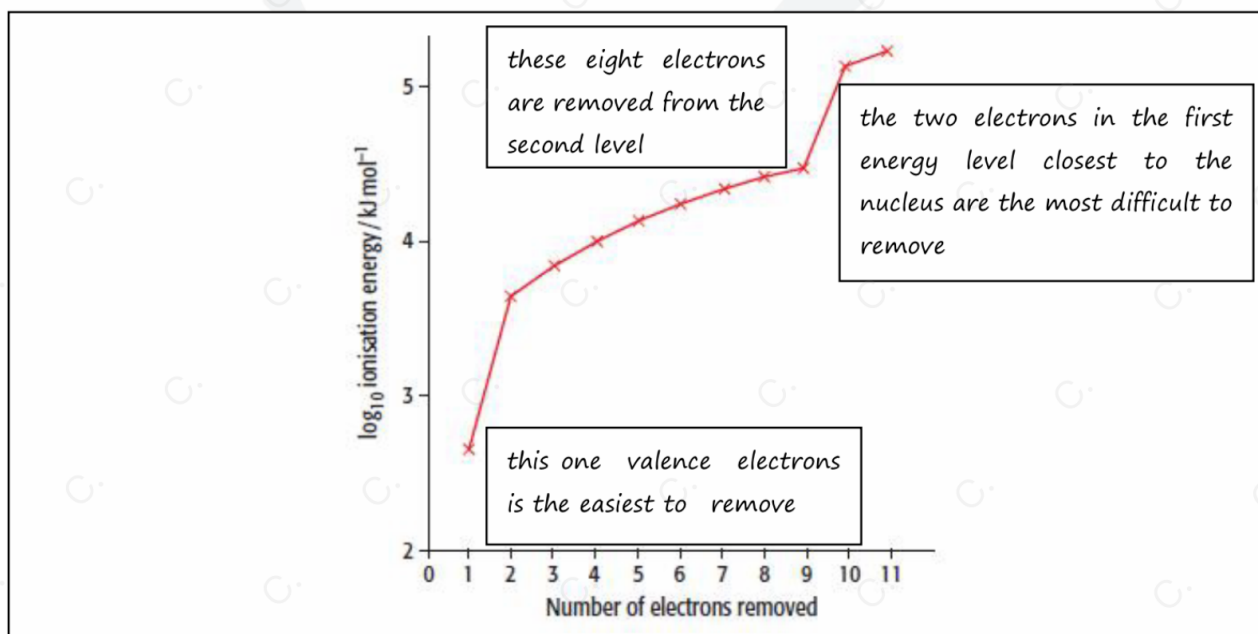
N $1s^2 2s^2 2p^3$ and O $1s^2 2s^2 2p^4$. In O, there is a pair of electrons are in the same 2p orbital, spin repulsion allows the electron to be removed more easily.

The **first** ionization energy for an element is the energy for the process:



The **second** ionization energy is: $M^+(g) \rightarrow M^{2+}(g) + e^-$

The **nth** ionization energy is: $M^{(n-1)+}(g) \rightarrow M^{n+}(g) + e^-$



(Figure 3.7 Cambridge International AS and A Level Chemistry textbook p36)

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A logarithmic scale (to the base 10) is used because the values of successive ionisation energies have such a large range.

1. There is an increase in successive ionization energies. The process becomes more difficult as there is increasing nuclear attraction, electrons are closer to the nucleus and with less shielding. And the proton to electron ratio increases at the same time.

2. There is a large jump after first ionisation energy, because the first electron is in the third shell. And second electron enters an inner shell which is closer to nucleus and with less shielding (greater nuclear attraction). There is another jump between 9th ionisation energy and 10th ionisation energy, again the 10th electron enter the lowest energy shell, which is the closest to nucleus and with no shielding (the greatest nuclear attraction).

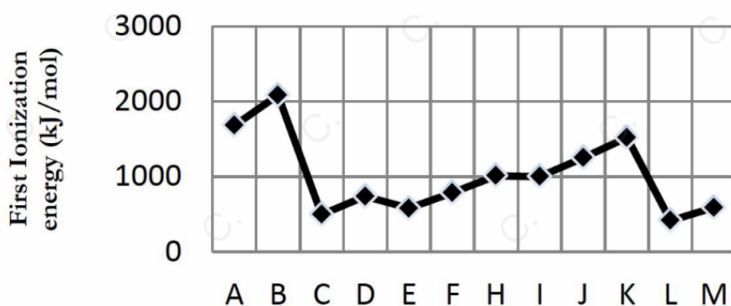
Example 5. (Source:2018, CCC, a, 20)

Which of the following accurately represents a trend in atomic radius?

- A) $F > Cl > Br$ B) $F > O > N$ C) $Cl^- > Na^+ > Mg^{2+}$
 D) $Ca^{2+} > K^+ > Ca$ E) $O^{2-} > S^{2-} > Cl$

Exercise 5. (source: 2013, CCC, a, 21)

Below is a selection of unidentified consecutive elements on the period table (the atomic number increases by 1 from A to B and so on).



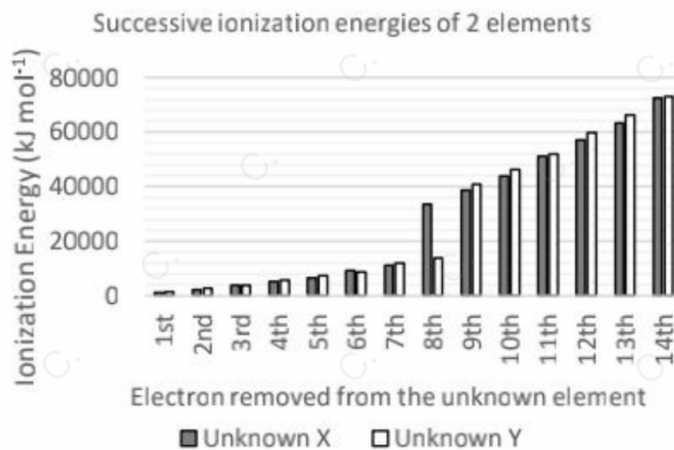
An element that is likely to be a halogen is: _____ (source: 2013, CCC, a, 21)

- A) A B) B C) C D) H E) M

Example 6 . (source: 2020, CCC, a, 6)

Given the graph of the successive ionization energies for two unknown atoms, which combination provides the most likely identity of X and

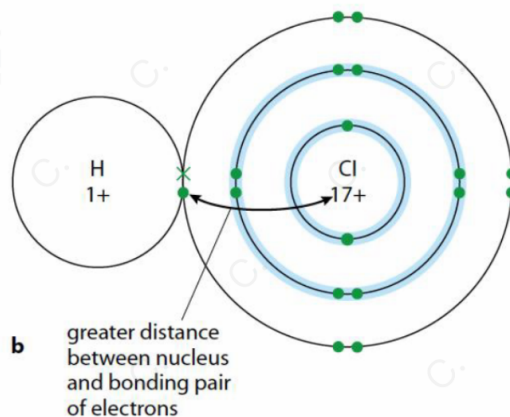
| Unknown: | X | Y |
|----------|----|----|
| A) | Al | Si |
| B) | Kr | Rb |
| C) | Cl | Ar |
| D) | Se | Br |
| E) | Rb | Sr |



Y?

3.3.5 Electronegativity

Definition – it is the ability of an atom to attract a pair of electrons in a covalent bond.



(Figure 3.8 page 96 chemistry for IB Diploma coursebook 2nd editions)

- The electronegativity increases across the period
- The electronegativity decreases down the group
- Noble gases are not assigned the electronegativity values



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The scale for measuring electronegativities goes from 0.7 to 4.0 (with 4.0 being the highest value).

The element with the largest electronegativity is fluorine. This is because fluorine has the highest effective nuclear charge and the least amount of shielding.

While the noble gases do have a higher nuclear charge, they are unable to react with other elements due to their electron configuration (this will be covered in Chapter 6).

By definition, the attraction for other electrons has to be in a chemical reaction. The element with the smallest electronegativity is cesium. This is because its electrons are highly shielded and experience a small effective nuclear charge (see Figure 3.9)

| | | | | | | | |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|--|
| H | | | | | | | |
| 2.1 | | | | | | | |
| Li | Be | B | C | N | O | F | |
| 1.0 | 1.5 | 2.0 | 2.5 | 3.0 | 3.5 | 4.0 | |
| Na | Mg | Al | Si | P | S | Cl | |
| 0.9 | 1.2 | 1.5 | 1.8 | 2.1 | 2.5 | 3.0 | |
| K | Ca | Ga | Ge | As | Se | Br | |
| 0.8 | 1.0 | 1.6 | 1.8 | 2.0 | 2.4 | 2.8 | |
| Rb | Sr | In | Sn | Sb | Te | I | |
| 0.8 | 1.0 | 1.7 | 1.8 | 1.9 | 2.1 | 2.5 | |
| Cs | Ba | Tl | Pb | Bi | Po | At | |
| 0.7 | 0.9 | 1.8 | 1.9 | 1.9 | 2.0 | 2.2 | |

Electronegativity values for the first six periods of representative elements

Figure 3.9

Example 7: Rank the following by increasing electronegativity: N, P, O

Exercise 7: Explain why H has an electronegativity so much larger than Li.

Point 4: Bonding and structure

4.1 Covalent bond

When two non-metal atoms combine, they share one, or more, pairs of electrons. A shared pair of electrons is called a single covalent bond, or a bond pair. A Covalent molecule contain only covalent bonds. In this part, we will learn the geometries of molecules and their electronic structures.

4.1.1 Lewis structure

In the Lewis structure (also known as electron dot structure) all the valence electrons are shown. Electrons may be shown individually as dots or crosses, or a line may be used to represent a pair of electrons.



A Lewis structure is complete when all atoms in the molecule are connected through covalent bonds and all valence electrons are distributed within the structure as either bonding electrons or lone pairs, such that all atoms obey the octet rule.

The **octet rule** states that atoms share electrons with neighbouring atoms to achieve a total of 8 valence electrons, known as an octet. This is based on the concept of fully filling the s and p subshells to achieve a stable electron configuration. Thus, the concept of octet rule is strictly limited to elements in the 2nd period.

For elements from the 3rd period onwards, it is possible for atoms to have more than 8 electrons in the valence shell, known as **hypervalence**.

To construct a Lewis structure, we may follow the 4 steps below:

1. Find the total number of valence electrons required for each atom to attain noble gas configuration.
2. Find the actual number of valence electrons present, accounting for the overall charge.

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3. Subtract the actual number of valence electrons from the total number of valence electrons required to find the number of valence electrons that must be shared. The total number of bonds will be half the number of valence electrons to be shared.

4. After the bonds are drawn, add lone pairs to each atom until it has a full octet.

Let us demonstrate how to apply these rules by drawing the Lewis structure of BF_4^- :

1. All 5 atoms require 8 electrons to achieve noble gas configuration, thus a total of $5 \times 8 = 40$ valence electrons are required.

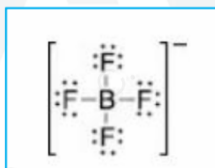
2. Boron has 3 valence electrons while each fluorine has 7 valence electrons.

Accounting for the overall -1 charge, there are a total of $3 + (4 \times 7) + 1 = 32$ valence electrons present.

3. The number of valence electrons that needs to be shared is $40 - 32 = 8$.

8 valence electrons correspond to bonds.

4. After the 4 B-F bonds are drawn, boron already has a full octet. Each fluorine needs 6 more valence electrons, which should be added as 3 lone pairs.



Dots and crosses can be used in Lewis structures to indicate where the electrons originally came from.

Certain Lewis structures have many resonance forms. **Resonance** is to signify that there is more than one possible way in which the valence electrons can be arranged in a Lewis structure. Resonance structures are usually shown with a double headed arrow between them. The resonance hybrid averages the bond characteristics over the molecule, resulting in it having a lower energy than any single contributing

structure. For example, carboxylate anion has 3 resonance forms, as shown in Figure

4.1. All 3 C–O bonds in carboxylate are in fact equivalent.

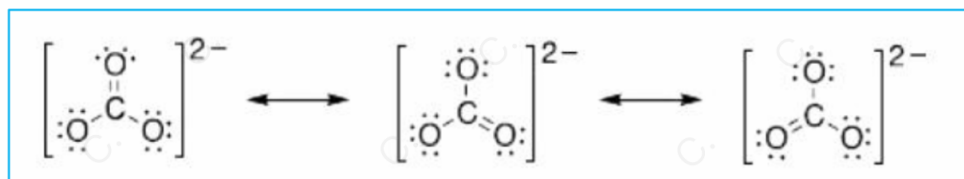


Figure 4.1

4.1.2 Co-ordinate bonding (dative covalent bonding)

A **co-ordinate bond** (or **dative covalent bond**) is formed when one atom provides both the electrons needed for a covalent bond. For dative covalent bonding we need:

- one atom having a lone pair of electrons
- a second atom having an unfilled orbital to accept the lone pair; in other words, an electron-deficient compound.

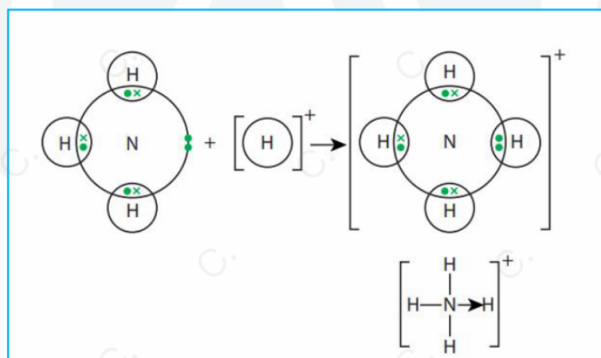


Figure 4.2 The formation of a co-ordinate bond in the ammonium ion

—《Cambridge International AS and A Level Chemistry Coursebook》P53

Example 8.(source, UKChO, 2019, 1)

(a) (i) Draw dot and cross diagrams for carbon dioxide and carbon monoxide.

4.2 VSEPR theory

The geometry of molecules may be predicted by **Valence Shell Electron Pair Repulsion (VSEPR)** theory. This approach allows us to find the approximate shapes of molecules for molecules with a central p-block atom. VSEPR theory assumes that the regions with enhanced electron density, such as bonding and lone electron pairs, take up positions as far apart as possible to minimise the repulsions between them. This theory is a basic theory that does not account for steric factors and may not be used when the central atom is from the d-block.

Each of the following counts as a single **electron pair**: a lone pair, a single bond, a double bond, a triple bond, or a single electron (as in a free radical).

Electron pairs repulsions vary as follows:

- ✓ Lone pair– lone pair > lone pair – bonding pair > bonding pair – bonding pair (LP-LP > LP-BP > BP-BP)
- ✓ The smaller the angle between electron pairs, the greater the repulsion
- ✓ Triple bonds > double bonds > single bond

For example, bond angles decrease in the following order: $\text{CH}_4 > \text{NH}_3 > \text{H}_2\text{O}$

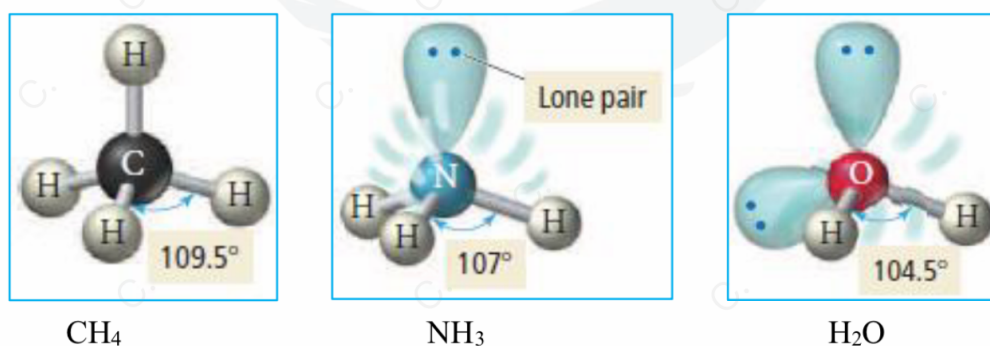


Figure 4.3

4.2.1 Steps for determining the geometry using VSEPR theory:

1) Determine the no. of electron pairs from the Lewis structure of the molecule.


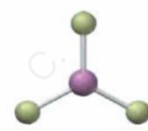
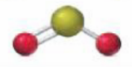
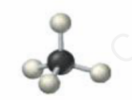
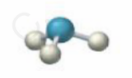
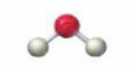
If the Lewis structure contains resonance structures, use any one of the resonance structures to determine the number of electron pairs.



When there are multiple bonds, it is treated as a single bond.

2) Predict the geometry of electron pairs around each atom by assuming that the pairs are oriented in space as far away from one another as possible.

The table of Electron and Molecular Geometries

| Electron Groups* | Bonding Groups | Lone Pairs | Electron Geometry | Molecular Geometry | Approximate Bond Angles | Example |
|------------------|----------------|------------|-------------------|--------------------|-------------------------|---|
| 2 | 2 | 0 | Linear | Linear | 180° | $\text{:}\ddot{\text{O}}=\text{C}=\ddot{\text{O}}\text{:}$  |
| 3 | 3 | 0 | Trigonal planar | Trigonal planar | 120° | $\begin{array}{c} \text{:}\ddot{\text{F}}\text{:} \\ \\ \text{:}\ddot{\text{F}}-\text{B}-\ddot{\text{F}}\text{:} \end{array}$  |
| 3 | 2 | 1 | Trigonal planar | Bent | <120° | $\text{:}\ddot{\text{O}}=\ddot{\text{S}}-\ddot{\text{O}}\text{:}$  |
| 4 | 4 | 0 | Tetrahedral | Tetrahedral | 109.5° | $\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{H} \\ \\ \text{H} \end{array}$  |
| 4 | 3 | 1 | Tetrahedral | Trigonal pyramidal | <109.5° | $\begin{array}{c} \text{H} \\ \\ \text{H}-\text{N}-\text{H} \\ \\ \text{H} \end{array}$  |
| 4 | 2 | 2 | Tetrahedral | Bent | <109.5° | $\text{H}-\ddot{\text{O}}-\text{H}$  |



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| | | | | | | | |
|---|---|---|----------------------|----------------------|------------------------------------|--|--|
| 5 | 5 | 0 | Trigonal bipyramidal | Trigonal bipyramidal | 120° (equatorial) 90° (axial) | | |
| 5 | 4 | 1 | Trigonal bipyramidal | Seesaw | <120° (equatorial) <90° (axial) | | |
| 5 | 3 | 2 | Trigonal bipyramidal | T-shaped | <90° | | |
| 5 | 2 | 3 | Trigonal bipyramidal | Linear | 180° | | |
| 6 | 6 | 0 | Octahedral | Octahedral | 90° | | |
| 6 | 5 | 1 | Octahedral | Square pyramidal | <90° | | |
| 6 | 4 | 2 | Octahedral | Square planar | 90° | | |

4.2.2 The formula of VPN

The geometry of AX_mL_n molecular depends on the number of the valence shell electron Pairs (VPN) surrounding central atom A.

Where, A is the central atom, X is the ligand atom, L is the lone pair electron, m is the number of Ligand atoms, n is the number of lone pair electrons.

The formula of VPN (the number of the Valence electronic pairs):

- ✓ Molecular: $VPN = 1/2$ [valence electron number of A + the number of electrons provided by X bonding with central atom]
- ✓ Ion: $VPN = 1/2$ [valence electron number of A + Number of valence electrons provided by X - charge numbers of the ion]

where,

→Valence electron number of A = family number of A

For example, IIA (2), Boron (3), Carbon (4), Nitrogen (5), Oxygen (6), Halogen (7), Rare gas (8)

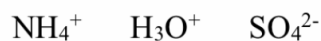
→The number of valence electrons provided by X: H and halogen are recorded as 1, and oxygen and sulfur are recorded as 0.

Fomula : the number of the lone pair electrons : n $n = VPN - m$

Or Molecular : $n = (\text{valence electron number of A} - m) / 2$

Ion : $n = (\text{valence electron number of A} - m - \text{charge numbers of the ion}) / 2$

Example 9: Calculate the VPN values of the following ions



Exercise 9. Determine the geometry of the molecule BrF_3



4.3 Metallic Bonding

The electrons in metallic are described as **delocalised** because they do not belong to any one metal atom but, rather, are able to move throughout the structure. The metallic bond is resulting from the attraction between the positive metal ions and the negatively charged delocalised electrons:

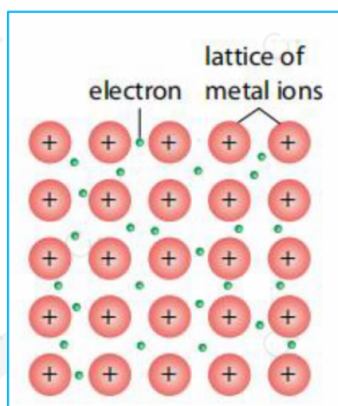


Fig 4.4 A metallic structure

This is a giant structure – there are no individual molecules

4.4 Ionic bond

The strong force of attraction between the positive and negative ions in the ionic crystal lattice results in an **ionic bond**. An ionic bond is sometimes called an **electrovalent bond**. In an ionic structure, the ions are arranged in a regular repeating pattern. As a result of this, the force between one ion and the ions of opposite charge that surround it is very great. In other words, ionic bonding is very strong. The classic example of an ionic compound is magnesium oxide MgO . (see fig 3)



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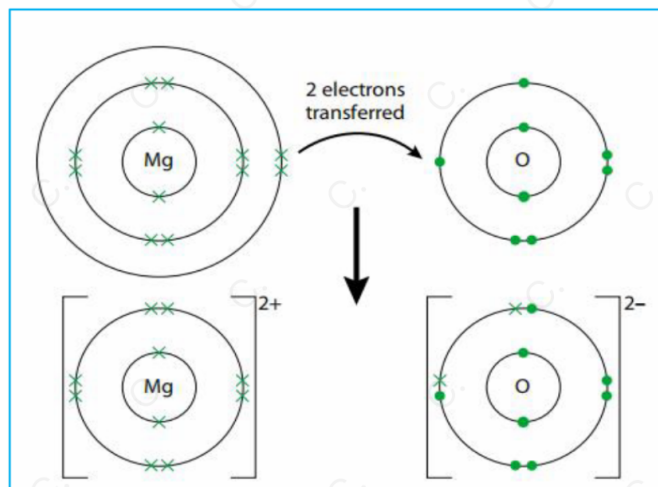


Fig 4.5. Electron transfer in ionic bonding

Example 10: Determine the number of the lone pair electrons surrounding the central atom and infer the molecular geometric of SF_4

Exercise 10: Determine the number of the lone pair electrons n surrounding the central atom and infer the geometric geometry of SO_3

Point 5: Intermolecular forces

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5.1 Molecular polarity

Whether a molecule is polar, or not, depends both on the relative electronegativities of the atoms in the molecule and on its shape. If the individual bonds are polar then it does not necessarily follow that the molecule will be polar as the resultant dipole may cancel out all the individual dipoles.

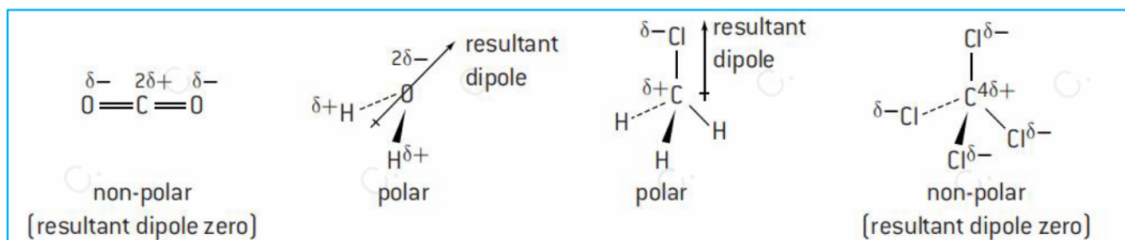


Fig5.1 《IB Chemistry Study guide》 P29

5.2 Intermolecular forces

The forces within molecules due to covalent bonding are strong. However, the forces between molecules are much weaker. We call these forces **intermolecular forces**. There are three types of intermolecular force:

- van der Waals' forces (which are also called 'London dispersion forces' and 'temporary dipole-induced dipole forces')
- permanent dipole-dipole forces
- hydrogen bonding.

5.2.1 London dispersion forces

Even in non-polar molecules the electrons can at any one moment be unevenly spread. This produces temporary instantaneous dipoles. An instantaneous dipole can induce another dipole in a neighbouring particle resulting in a weak attraction between the two particles. London dispersion forces increase with increasing mass.

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| | increasing London dispersion forces | | | |
|------------|-------------------------------------|---------------------------------------|---------------------------------------|--|
| | → | | | |
| M_r | CH ₄ 16.0 | C ₂ H ₆ 30.0 | C ₃ H ₈ 44.0 | C ₄ H ₁₀ 58.0 |
| b. pt / °C | -162 | -88.6 | -42.2 | -0.5 |

Fig5.2 《IB Chemistry Study guide》 P29

5.2.1 Dipole–Dipole forces

Polar molecules are attracted to each other by electrostatic forces. Although still relatively weak the attraction is stronger than London dispersion forces.

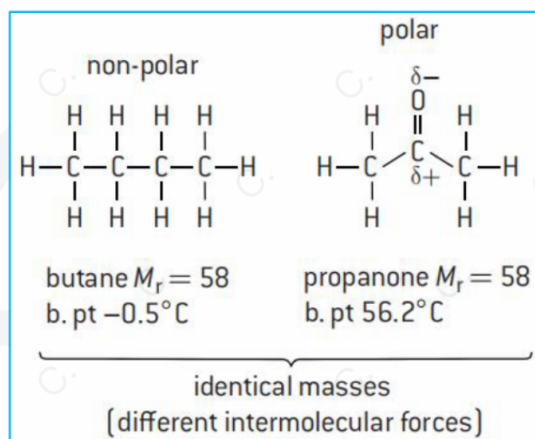


Fig5.3 《IB Chemistry Study guide》 P29

5.2.2 Hydrogen bonding

When a hydrogen atom is covalently bonded to a very electronegative atom (eg: N, O, F), the bond is very highly polarised. The δ^+ charge on the hydrogen atom is high enough for a **Hydrogen bond**. It is the strongest type of intermolecular force.

The force of attraction in hydrogen bond is about one-tenth of the strength of a normal covalent bond. For maximum bond strength, the angle between the covalent bond to the hydrogen atom and the hydrogen bond is usually 180°

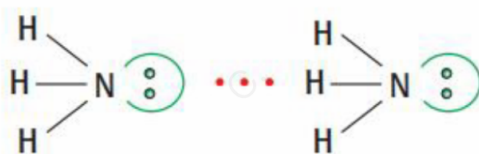


Figure 5.4 A hydrogen bond is represented by a line of dots.

⇒ Hydrogen bonding can:

- influence the solubility of substances in water (molecules that are able to hydrogen bond are soluble in water).
- increase the boiling point of substances.

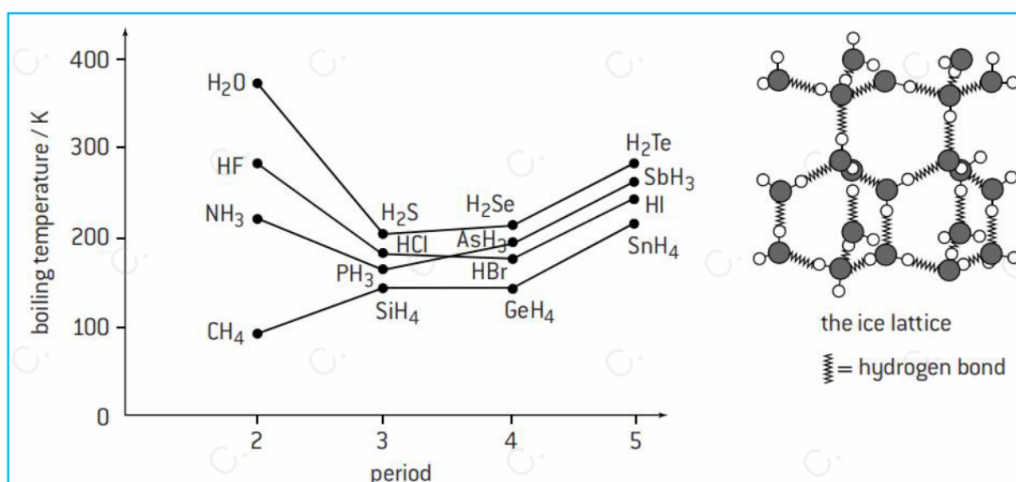


Fig5.5 《IB Chemistry Study guide》 P29

5.3 Compare the boiling points of substances

➤ Ionic crystals

Ionic crystals are compounds that contain ionic bonds, like NaCl—a crystal of sodium chloride consists of a giant lattice of Na⁺ and Cl⁻ ions. All the Na⁺ ions in the crystal attract all the Cl⁻ ions. These electrostatic forces are strong, so it is difficult to break apart the **lattice structure**. Ionic compounds usually have high melting points and boiling points.

⇒ The melting boiling point of ionic compounds is directly proportional to the strength of their ionic bonds:

- The shorter the ion radius, the more difficult the ionic bond is to break, and the higher the melting boiling point of ionic compounds.
- The greater the charge of ions, the stronger the ionic bond, and the higher the melting boiling point of ionic compounds.

For example, Magnesium oxide has a much higher melting point than sodium chloride because the electrostatic attractions between the $2+$ and $2-$ ions in the magnesium oxide lattice are much stronger than those between the $1+$ and $1-$ ions in sodium chloride. A higher temperature is required to provide sufficient energy to separate the ions in magnesium oxide.

➤ Atomic crystals

Atomic crystal is a crystal directly composed of atoms contain ionic bonds, like diamond、 silicon.

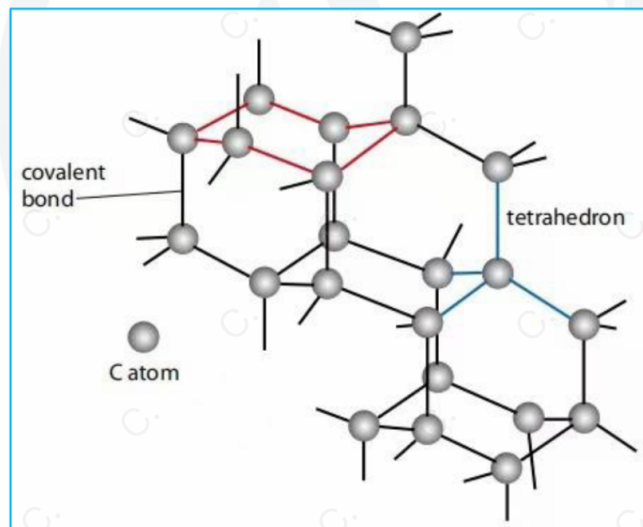


Figure 5.6 Part of the diamond structure

⇒ **The shorter the bond length between atoms, the more stable the covalent bond, the higher the melting boiling point of the material, and vice versa.**

➤ Molecular crystals

When a molecular crystal melts, it destroys the intermolecular force- van der Waals force {orientation force, induction force and The London dispersion force}, rather



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than the destruction of "chemical bond", so the melting boiling point of molecular crystals is generally low. The dispersion force is related to the molecular weight. **The greater the molecular weight, the greater the intermolecular force in molecular crystals, the higher the melting boiling point of substances**

However, the melting boiling point of molecular **crystals with hydrogen bonds will be abnormally high**, such as H_2O , HF , etc.

■ In most cases, the order of melting boiling point is atomic crystal > ionic crystal > molecular crystal

➤ Metals

Most metals have high melting points and high boiling points. The more valence electrons of metal atoms in metal crystals, the smaller the atomic radius, the stronger the electrostatic interaction between metal cations and free electrons, the stronger the metal bond and the higher the melting boiling point.

Example 11. (source: 2019, CCC, a, 5)

The melting point of CaS is higher than that of KCl . Explanations for this observation include which of the following?

- I. Ca^{2+} is more positively charged than K^+ .
- II. S^{2-} is more negatively charged than Cl^- .
- III. The K^+ ion is smaller than the Ca^{2+} ion.

- A. II only
- B. I and II only
- C. I and III only
- D. II and III only
- E. I, II, and III



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Exercise 11. (*source: 2017, CCC, a, 3*)

In which of the following situations could hydrogen bonding occur between H₂O and the solute? (*source: 2017, CCC, a, 3*)

- A. ammonia gas dissolved in water
- B. hydrogen gas dissolved in water
- C. carbon dioxide gas in water
- D. methane gas dissolved in water
- E. hydrogen sulfide gas dissolved in water



Summary

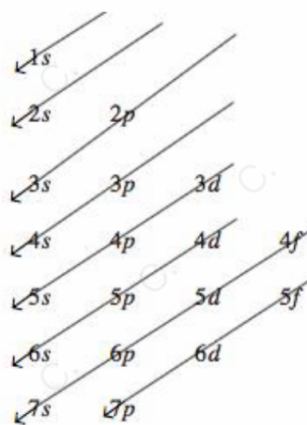
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1. atom structure:

- 1) the number of protons、 the number of neutrons、 the number of electrons、 mass number、 atomic number.
- 2) Isotopes: Isotopes are atoms of the same element which have the same number of _____, but different number of neutrons. Isotopes have the same _____ properties (they react in the same way) , but different _____ properties (for example, melting point or boiling point).

2. Electron configuration

- 1) the principle quantum number ($n=1, 2, 3, 4\dots$) correspond to K、 L、 M、 N... electron layers.
- 2) the angular quantum number ($l=0,1,2,3,\dots$) correspond to s、 p、 d、 f ...orbits.
- 3) The electric configuration:
 - ✓ **Aufbau principle:** the electrons fill the sublevels from the lowest level, which gives the lowest possible energy. **According to the Aufbau Principle** in quantum mechanics, the electrons are arranged according to the energy levels of high and low energy levels, and the general order is as follows:



$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 5f < 6d \dots < ns < \underline{\hspace{1cm}} < \underline{\hspace{1cm}} < \underline{\hspace{1cm}} f < \underline{\hspace{1cm}} d < np.$



3. Summary of Periodic Trends

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1) Going from left to right across a period, nuclear charge increases, while shielding effect is unaffected. As a result:

- atomic radius _____.
- ionization energy increases.
- Electron affinity _____.
- electronegativity _____.

2) Going from top to bottom down a group, nuclear charge is unaffected while shielding effect increases (see Figure 6.1). As a result:

- atomic radius increases.
- ionization energy _____.
- electron affinity _____.
- electronegativity _____.

4. Chemical bond

Ions are formed when atoms gain or lose electrons.

_____ **bonding** involves an attractive force between positively and negatively charged ions in an ionic lattice.

A _____ **bond** is formed when atoms share a pair of electrons.

When atoms form covalent or ionic bonds each atom or ion has a full outer electron shell of electrons. (Some covalent compounds may be electron deficient or have an 'expanded octet'.) Dot-and-cross diagrams can be drawn to show the arrangement of electrons in ionic and covalent compounds. The reactivities of covalent bonds can be explained in terms of bond energy, bond length and bond polarity.

Electronegativity differences can be used to predict the type of weak _____ forces between molecules.

Metallic bonding can be explained in terms of a lattice of positive ions surrounded by mobile electrons.

5. VSEPR theory:

Electron pairs repel one another and stay as far apart as possible, thus causing



molecules to assume specific shapes.

the geometry of a molecule is determined by the number of electron pairs on the central atom.

Electron pairs repulsions vary as follows:

- ✓ ___ pair - ___ pair > ___ pair - ___ pair > ___ pair - ___ pair
(___ > ___ > ___)
- ✓ The smaller the angle between electron pairs, the _____ the repulsion
- ✓ Triple bonds > double bonds > single bond

6. Determination of the Geometry of Molecules Having Single Bonds

Formula: AX_mL_n

(1) $VPN = BP + LP$ 或 $VPN = m + n$ (m is the number of ligands, m = the number of BP in single Bonds, n = the number of the lone electron pairs)

Molecular: $VPN = 1/2$ [_____ number of A + the number of electrons provided by X bonding with central atom]

Ion: $VPN = 1/2$ [_____ number of A + Number of valence electrons provided by X - charge numbers of the ion]

where,

→ _____ number of A = family number of A

For example, IIA (2), Boron (3), Carbon (4), Nitrogen (5), Oxygen (6), Halogen (7), Rare gas (8)

→ The number of valence electrons provided by X: H and halogen are recorded as _____, and oxygen and sulfur are recorded as _____.


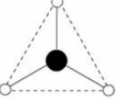
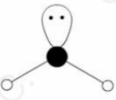
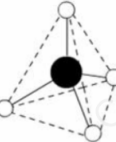
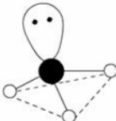
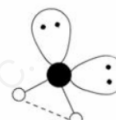
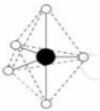
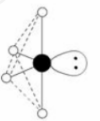


(2) **the number of the lone pair electrons** : $n =$ _____

For Molecular : $n =$ (_____ of A - m) / 2

For Ion : $n =$ (_____ number of A - m - charge numbers of the ion) / 2

7. The electron geometry and molecular geometry of the central atoms

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| VPN (价层电子对数) | m | n | AX_mL_n | Electron geometry (电子对空间排布) | molecular geometric (分子空间构型) | For example |
|-----------------|---|---|-----------|---|------------------------------------|-------------|
| 2 | 2 | 0 | AX_2 | Linear  | linear | $BeCl_2$ |
| 3 | 3 | 0 | AX_3 | trigonal  | trigonal planar | BF_3 |
| | 2 | 1 | AX_2L | trigonal  | — | $SnCl_2$ |
| 4 | 4 | 0 | AX_4 | tetrahedral  | — | CH_4 |
| | 3 | 1 | AX_3L | tetrahedral  | trigonal pyramid | NH_3 |
| | 2 | 2 | AX_2L_2 | tetrahedral  | V-shaped or — | H_2O |
| 5 | 5 | 0 | AX_5 | trigonal bipyramid  | trigonal bipyramid | PCl_5 |
| | 4 | 1 | AX_4L | trigonal bipyramid  | distorted tetrahedron (or see saw) | SF_4 |
| | 3 | 2 | AX_3L_2 | trigonal bipyramid  | — | ClF_3 |
| | 2 | 3 | AX_2L_3 | trigonal bipyramid  | Linear | XeF_2 |



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| | | | | | | |
|---|---|---|-----------|----------------|----------------|---------|
| | | | | | | |
| 6 | 6 | 0 | AX_6 | octahedral | octahedral | SF_6 |
| | 5 | 1 | AX_5L | octahedral | square pyramid | ClF_5 |
| | 4 | 2 | AX_4L_2 | octahedral | — | XeF_4 |

8. Relationship among molecule geometry 、 molecular polarity and molecular dipole moment.

Generally, if the molecular geometry is symmetrical, the molecule is non-polar and the dipole moment is 0.

If the molecular geometry is unsymmetrical, the molecule is polar, and the dipole moment is not zero.

7. Intermolecular forces

Three types of relatively weak intermolecular forces are hydrogen bonding, permanent dipole-dipole forces and van der Waals' forces.

- The physical properties of substances may be predicted from the type of bonding present.
- Substances with ionic bonding have high melting and boiling points, whereas simple molecules with covalent bonding have low melting points.
- The presence of hydrogen bonding in a molecule influences its melting point and boiling point.