# Introduction to organic chemistry Branches of Chemistry

#### • Primary

- Physical Chemistry
  - study of the physical basis of phenomena related to the chemical composition and structure of substances
  - the theories of physics to atoms and subatomic particles.
  - When physical chemistry is applied to the chemical interaction between atoms and subatomic particles, the study is known by the name, quantum mechanics.
  - It is a relatively vast field that deals with intermolecular forces, rates of chemical reactions as well the conductivity of different materials

# **Branches of Chemistry**

- Primary...
  - Inorganic Chemistry (study, structure, composition and behavior of compounds of mineral origin).
    - the study the properties and reactions of compounds that do not contain carbon i.e.
    - All the substances other than the carbon-hydrogen compounds are classified under the group of inorganic substances.
    - Oxides, sulphides and carbonates form the important classes of inorganic compounds.

# **Branches of Chemistry**

- Primary ...
  - Organic Chemistry (study of hydrocarbons and their derivatives)
    - This branch of chemistry deals with the study of the organic matter.
    - The substances that primarily consist of carbon and hydrogen are termed as organic.
    - The discipline that deals with the study of the structure, composition and the chemical properties of organic compounds

(more details later ....)

# Secondary Branches of Chemistry

- Analytical
  - the analysis of the chemical properties of natural and man-made materials (qualitative and quantitative)
  - It has played critical role in the sciences ranging from the development of concepts and theories to a variety of practical applications, such as biomedical applications, environmental monitoring, quality control of industrial manufacturing and forensic science
  - Examples include analysis of drinking water, analysis of damage from industrial fires, chemical risk management etc

# Secondary Branches

Industrial

- Chemistry that is used in industrial applications e.g.
  - Synthetic fibre like rayon, nylon, etc.
  - Plastics like bakelite, teflon, polythene etc.
  - Paints, varnishes, enamels, dyes etc.
  - Cement, glass and ceramics and extraction of metals like silver, magnesium, gold, iron etc.
  - Extraction and Purification of Crude oil
  - Production of biogas from industrial waste & sewage
- Biochemistry
  - the study of the chemical processes in living organisms.
  - It deals with the structure and function of cellular components such as proteins, carbohydrates, lipids (fats), nucleic acids (e.g. DNA) and other biomolecules.

# Secondary Branches

#### • Environmental Chemistry

- the scientific\_study of the chemical and biochemical phenomena that occur in natural places.
- A contaminant is a substance present in nature at a level higher than typical levels or that would not otherwise be there. These can include:
  - Heavy metal contamination of land by industry. These can then be transported into water bodies and be taken up by living organisms.
  - Nutrients leaching from agricultural land into water courses, which can lead to algal blooms and eutrophication.
  - Urban runoff of pollutants washing off impervious surfaces (roads, parking lots, and rooftops) during rain storms.

# **Specialised Branches of Chemistry**

- Agricultural Chemistry the study of both chemistry and biochemistry which are important in agricultural production, the processing of raw products into foods and beverages, and in environmental monitoring and remediation
- **Cosmochemistry** the origin and development of the elements and their isotopes, primarily within the Solar System.
- **Geochemistry** study of the chemical composition of the Earth and other planets, chemical processes and reactions that govern the composition of rocks and soils, and the cycles of matter and energy that transport the Earth's chemical components in time and space, and their interaction with the hydrosphere and the atmosphere.

# Specialised Branches of Chemistry

- Food Chemistry the study of chemical processes and interactions of all biological and nonbiological components of foods.
- Forensic chemistry is the application of chemistry to law enforcement or the failure of products or processes. Many different analytical methods may be used to reveal what chemical changes occurred during an incident, and so help reconstruct the sequence of events.

# Specialised Branches of Chemistry

• Femtochemistry - the science that studies chemical reactions on extremely short timescales, approximately 10<sup>-15</sup> seconds (one femtosecond, hence the name) in order to reveal details about the intermediate products that form during chemical reactions, which cannot be deduced from observing the starting and end products.

# Specialised Branches of Chemistry

• Theoretical chemistry- the mathematical characterization of bulk chemistry in various phases (e.g. the study of chemical kinetics) and the study of the applicability of more recent math developments to the basic areas of study (e.g. for instance the possible application of principles of topology to the study of electronic structure.). It is also the use of physics to explain or predict chemical phenomena. In recent years, it has consisted primarily of quantum chemistry, i.e., the application of quantum mechanics to problems in chemistry.

# Specialised Branches of Chemistry

• **Computational chemistry** is a branch of chemistry that uses principles of computer science to assist in solving chemical problems. It uses the results of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules and solids. While its results normally complement the information obtained by chemical experiments, it can in some cases predict hitherto unobserved chemical phenomena. It is widely used in the design of new drugs and materials

# Specialised Branches of Chemistry

- Radiation/ Nuclear Chemistry is a subfield of chemistry dealing with radioactivity, nuclear processes and nuclear properties
- **Sonochemistry** the branch which deals with the study of sonic waves and their properties on chemical systems i.e. Any chemical reaction that takes place, or is initiated by sound or ultrasound)
- Solid State Chemistry the study of the synthesis, structure, and physical properties of solid materials with emphasis on New phases, phase diagrams, structures, Optical properties, Electrical properties and Magnetic properties)

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# Specialised Branches of Chemistry

- Soil Chemistry is the study of the chemical characteristics of soil. Soil chemistry is affected by mineral composition, organic matter and environmental factors
  - Soil Mineralogy and Ion Fixation
  - Soil Acidity and Alkalinity
  - Soil Organic Matter
  - Soil Colloid Surface Charge and Dispersion

# Specialised Branches of Chemistry

• Electrochemistry - is a branch of chemistry that studies chemical reactions which take place in a solution at the interface of an electron conductor (a metal or a semiconductor) and an ionic conductor (the electrolyte), and which involve electron transfer between the electrode and the electrolyte or species in solution

# Specialised Branches of Chemistry

- Nanochemistry the use of synthesis to make nanoscale building blocks of desired shape, size, composition and surface structure, charge and functionality with an optional target to control self-assembly of these building blocks at various scale-lengths
- Macromolecular chemistry The chemistry of macromolecules (e.g., proteins, nucleic acids e.g. DNA and RNA) and polymers (nylon, polyethylene, etc)

# Specialised Branches of Chemistry

- Medicinal chemistry (and pharmaceutical chemistry) involved with designing, synthesizing and developing pharmaceutical drugs.
- Medicinal chemistry involves the identification, synthesis and development of new chemical entities suitable for therapeutic use. It also includes the study of existing drugs, their biological properties, and their quantitative structure-activity relationships.
- Pharmaceutical chemistry is focused on quality aspects of medicines and aims to assure fitness for the purpose of medicinal products

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# Back to Organic Chemistry

- Importance of Organic Chemistry
- Organic Chemistry and Industry
- History of Organic Chemistry (as a subject) not "History of Organic Compounds" – i.e. birth of the word "Organic"

## Importance of Organic Chemistry

- Just about all of the molecules that make life possible: proteins, enzymes, vitamins, lipids (fats), carbohydrates, and nucleic acids—contain carbon, so the chemical reactions that take place in living systems, including our own bodies, are organic reactions.
- Most of the compounds found in nature—those we rely on for food, medicine, clothing (cotton, wool, silk), and energy (natural gas, petroleum) are organic as well.

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# Importance of Organic Chemistry

- Organic chemistry is a discipline within chemistry which involves the scientific study of the structure, properties, composition, reactions, and preparation (by synthesis or by other means) of hydrocarbons and their derivatives.
- These compounds may contain any number of other elements, including hydrogen, nitrogen, oxygen, the halogens as well as phosphorus, silicon and sulfur.

## Importance of Organic Chemistry

- Important organic compounds are not, however, limited to the ones we find in nature. Chemists have learned to synthesize millions of organic compounds never found in nature, including synthetic fabrics, plastics, synthetic rubber and medicines.
- Many of these synthetic compounds prevent shortages of naturally occurring products.
- Currently, there are about 16 million known organic compounds, and many more are possible

# **Organic chemistry and industry**

- Some simple compounds are made both from oil and from plants.
- The common alcohol, ethanol, is used as a starting material to make other compounds in industry is largely made by the catalytic hydration of a gas ethylene from crude oil.
- But ethanol is also used as a fuel, and is made by fermentation of sugar cane wastes

# **Plastics and Polymers**

- Plastics and polymers (e.g. PVC, polyester) take much of the production of the petrochemical industry (in addition to fuel for vehicles).
- The products of this enormous industry are everything made of plastic including solid plastics for household goods and furniture, fibres for clothes (over 24 million tonnes per annum), elastic polymers for car tyres, light bubble-filled polymers for packing.

## Detergents, soaps and Dyes...

- Companies like Unilever or Procter and Gamble which produce soap, detergent, cleaners, bleaches, polishes, and all the many essentials for the modern home.
- These products may be lemon and lavender scented but they too mostly come from the oil industry.
- There is a big market for intense colours for dyeing cloth, colouring plastic and paper, painting walls

# Synthetic Flavours

- Chemists produce synthetic flavourings such as 'smoky bacon' and even 'chocolate'.
- Meaty flavours come from simple heterocycles such as alkyl pyrazines (present in coffee as well as roast meat) and furonol, originally found in pineapples.
- Synthetic Organic Compounds are used to give caramel, meaty, 'cheese and onion' flavours etc.
- Mixtures of these and other synthetic compounds can be 'tuned' to taste like many roasted foods from fresh bread to coffee and barbecued meat

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# Natural and Artificial Sugars...

- Food chemistry includes much largerscale items than flavours. Sweeteners such as sugar itself are isolated from plants (beet and cane) on an enormous scale.
- Other sweeteners such as saccharin (discovered in 1879!) and aspartame (1965) are made on a sizeable scale.

### Pharmaceutical and Agro-Vet Industry

- The pharmaceutical businesses produce drugs and medicinal products of many kinds.
- The most famous modern insecticides are modeled on the natural pyrethrins, stabilized against degradation by sunlight by chemical and targeted to specific insects on specific crops in cooperation with biologists

# History of Organic Chemistry

- By the eighteenth century, scientists thought they had grasped the nature of difference between those from living organisms (covalent) and and those from inorganic (ionic) materials.
- In 1807, Jöns Jakob Berzelius gave names to the two kinds of materials: Compounds derived from living organisms were believed to contain an immeasurable vital force—the essence of life. These he called "organic."
- Compounds derived from minerals—those lacking that vital force—were "inorganic."

# History of Organic Chemistry

- Because chemists could not create life in the laboratory, they assumed they could not create compounds with a vital force.
- In 1828 when Friedrich Wöhler produced urea—a compound known to be excreted by mammals—by heating ammonium cyanate, an inorganic mineral

# History of Organic Chemistry

- Wohler was trying to make ammonium cyanate (NH<sub>4</sub>OCN) from silver cyanate (AgOCN) and ammonium chloride (NH<sub>4</sub>Cl).
- What he expected is described by the following equation.

 $AgOCN(aq) + NH_4Cl(aq) --> AgCl(s) + NH_4OCN(aq)$ 

# History of Organic Chemistry

- For the first time, an "organic" compound had been obtained from something other than a living organism.
- This discovery marked the end of the "vital force theory". Chemists at that time needed a new definition for "organic compounds."
- Organic compounds are now defined as "compounds that contain carbon" but more specifically, it is the study of <u>hydrocarbons (i.e.</u> compounds that contain carbon and hydrogen) and their derivatives.

# • The product he isolated from this reaction had none of the properties of cyanate compounds. It was a white, crystalline material that was identical to urea, $H_2NCONH_2$ , which could be isolated from urine $\begin{array}{c} \bigoplus_{H_4} \bigoplus_{OCN} & \bigoplus_{H_2N} \bigoplus_{Urea} \\ \bigoplus_{H_1} \bigoplus_{H_2} \bigoplus_{O-C \equiv N} \\ Molecular formular: NH_4OCN \\ Condensed Molecular formular: CH_4N_0 \\ \end{array}$

Ionic Salt

# Other definitions of Organic

- However the study of Carbon Monoxide (CO), Carbon Dioxide (CO<sub>2</sub>), carbonates (CO<sub>3</sub><sup>2-</sup>), cyanides (CEN<sup>-</sup>) etc is normally studied under "Inorganic Chemistry" due to their properties.
- Many organic compounds contain the elements oxygen, nitrogen and sulphur.

# The Structure of an Atom

- An atom consists of electrons, positively charged protons, and neutral neutrons
- Atomic number: numbers of protons in its nucleus
  - The atomic number is also the number of electrons that surround the nucleus of a neutral atom. For example, the atomic number of carbon is 6, which means that a neutral carbon atom has six protons and six electrons.
  - Because the number of protons in an atom does not change, the atomic number of a particular element is always the same—all carbon atoms have an atomic number of 6.

- Mass number: the sum of the protons and neutrons of an atom.
- Not all carbon atoms have the same mass number, because, even though they all have the same number of protons, they do not all have the same number of neutrons. For example, 98.89% of naturally occurring carbon atoms have six neutrons—giving them a mass number of 12 and 1.11% have seven neutrons—giving them a mass number of 13. These two different kinds of carbon atoms and are called isotopes.

- Isotopes have the same atomic number (i.e., the same number of protons), but different mass numbers because they have different numbers of neutrons.
- The chemical properties of isotopes of a given element are nearly identical.

- The atomic weight: the average weighted mass of the atomic masses over all the atoms in the sample
  - the ratio of the average mass of atoms of an element (from a given source) to 1/12 of the mass of an atom of carbon-12 (12.000000 amu).

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#### Atomic weights...For example for Carbon:

Naturally occurring isotope	Fractional abundance	Mass (amu)
<sup>12</sup> C	0.989	12.000000
<sup>13</sup> C	0.011	13.003355

- The sum of all the fractions of abundance of each naturally occurring isotopes (ie - add up column 2) should equal 1.0000 or 100%. (i.e. 98.9 % + 1.1 % = 100%)
- atomic mass of carbon
  - = (0.989)(12.000000 amu) + (0.011)(13.003355 amu)
  - = 11.8680 amu + 0.1430369 amu

= 12.011 amu



# Intramolecular forces: What is a bond?

- When two atoms are brought together, at some point, the attractions between the nuclei and the electrons are balanced against the repulsions between the nuclei and between the electrons.
- A **bond** is an attractive force between two atoms.
- The optimum distance between the nuclei where the net attractive forces are maximized is called the **bond length**. Pushing the nuclei closer together causes the potential energy to rise because of the increasing electrostatic repulsions

# The stability of the $H_2$ molecule can be explained on the basis of:

- Electron nuclei attractive interactions (electrons of one atom are attracted by the nucleus of the other).
- Electron electron repulsive interactions (electrons of one atom are repelled by the electrons of the other).
- Nucleus nucleus repulsive interactions (nucleus of one atom is repelled by the nucleus of the other).

# Types of Chemical Bonding

#### By transfer of electrons

• When the chemical bond occurs by the complete transfer of electron(s) from the atom(s) of one element to the atom or atoms of another element. The bond formed is called lonic (electrovalent) bond.

#### By sharing of electrons

• When the shared electrons are contributed by the two combining atoms equally, the bond formed is called Covalent bond.

# Ionic Bonding

- Attractive forces between opposite charges are called electrostatic attractions. A bond that is the result of only electrostatic attractions is called an ionic bond.
- The positively charged sodium ions and negatively charged chloride ions are independent species held together by the attraction of opposite charges.

# **Ionic Bonding**

- Thus, an **ionic bond** is formed when there is a *transfer of electrons*, causing one atom to become a positively charged ion and the other to become a negatively charged ion.
- Sodium chloride is an example of an ionic compound.
- **Ionic compounds** are formed when an element on the left side of the periodic table (an electropositive element) transfers one or more electrons to an element on the right side of the periodic table (an electronegative element)

# **Covalent Bonds**

- Instead of giving up or acquiring electrons, an atom can achieve a filled outer shell by sharing electrons. For example, two fluorine atoms can each attain a filled shell of eight electrons by sharing their unpaired valence electrons.
- A bond formed as a result of *sharing electrons* is called a **covalent bond**.

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# **Covalent Bonds**

- In covalent bonding, we picture atoms as sharing electrons to arrive at the same number of electrons as a noble gas. The shared electrons are counted as part of the total electrons for both of the atoms involved in the bond.
- Consider the simple example of the formation of the hydrogen molecule from two hydrogen atoms. Each hydrogen atom has one electron in its valence shell, and each would like to have two (helium configuration).

# Comparing Ionic and Covalent Compounds

- Ionic compounds have high melting points; a great deal of energy is needed to overcome the strong attractions between the oppositelycharged ions.
- Covalent compounds are generally gases, liquids, or low-melting solids.
- The covalent bonds within molecules are very strong, but the attractive forces between the separate molecules are fairly weak

# **Covalent Bonds**

 The simplest compound of carbon and hydrogen results from the combination of four hydrogen atoms with one carbon atom to produce methane, CH<sub>4</sub>.



## *Comparing lonic and Covalent Compounds*

• Some physical properties of Sodium Chloride and Hydrogen Chloride

Property	NaCl	НСІ
Formular Mass	58.44	36.46
Physical Appearance	White Solid	Colourless gas
Type of Bond	Ionic	Covalent
Melting Point (°C)	801	-115
Boiling Point (°C)	1413	-84.9

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# Polarity of Covalent Bonds

- A diatomic molecule has two atoms bonded to each other by a covalent bond.
- A covalent bond can be classified into:
  - Non Polar Covalent bond
  - Polar Covalent bond

# Non Polar Covalent Bond

- This type of covalent bond is described as a non-polar covalent bond.
- The bonds in the molecules H<sub>2</sub>, O<sub>2</sub>, Cl<sub>2</sub> etc., are non-polar covalent bonds.

# Non Polar Covalent bond

- When a covalent bond is formed between two atoms of the same element, the shared electron pair will lie exactly midway between the two atoms i.e. the electrons are equally shared by the atoms.
- The resulting molecule will be electrically symmetrical i.e., centre of the negative charge coincides with the centre of the positive charge.

# Polar Covalent Bond

 As the said electron pair do not lie exactly midway between the two atoms, the atom with higher affinity for electrons develops a slight negative charge and the atom with lesser affinity for electrons, a slight positive charge.

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# These are represented as δ+ and δ (delta meaning small) charges. Such molecules are called 'polar molecules'. δ+ δ- H-O: H-N-H H-C: H-O: H-N-H H H δ+ δ+ δ+







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# Shape of molecules on the basis of VSEPR theory

- The shape of the molecule is determined by both the total number of electron pairs (bonding and non-bonding) around the molecules central atom and the orientation of these electron pairs in the space around the central atom.
- In order to minimize the repulsion forces between them, electron pairs around the molecules central atom, tend to stay as far away from each other as possible.

#### Shape of molecules on the basis of valenceshell electron pair repulsion (VSEPR) theory

- Electron pairs around the molecule's central atom can be shared or can be lone pairs. The 'shared pairs' of electrons are also called bond pairs of electrons. The presence of lone pair(s) of electrons on the central atom causes some distortions in the expected regular shape of the molecule.
- The strength of repulsions between different electron pairs follows the order:
  - Lone pair Lone pair > Lone pair Shared pair > Shared pair Shared pair.

# Types of molecular structure relevant to organic chemistry

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- Linear: In a linear model, atoms are connected in a straight line. The bond angles are set at 180°.
- A bond angle is very simply the geometric angle between two adjacent bonds.
- For example, carbon dioxide has a linear molecular shape.



#### • Trigonal planar:

- In a molecule having three bond pairs of electrons around its central atom, the electron pairs form an equilateral triangular arrangement around the central atom.
- Just from its name, it can easily be said that molecules with the trigonal planar shape are somewhat triangular and in one plane (meaning a flat surface).

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# Trignal Planar Molecules (i.e. those with three bond pairs)

• Consequently, the bond angles are set at 120°. An example of this is boron trifluoride.



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• An example of a tetrahedral molecule is methane (CH<sub>4</sub>).



# Types of molecular structure relevant to organic chemistry

• **Tetrahedral:** *Tetra*- signifies four, and *-hedral* relates to a surface, so tetrahedral almost literally means "four surfaces." This is when there are four bonds all on one central atom, with no extra unshared electron pairs. In accordance with the VSEPR, the bond angles between the electron bonds are 109.5°.

# Types of molecular structure relevant to organic chemistry

• **Pyramidal (or trignal pyramidal):** Pyramidalshaped molecules have pyramid-like shapes. Unlike the linear and trigonal planar shapes but similar to the tetrahedral orientation, pyramidal shapes requires three dimensions in order to fully separate the electrons. Here, there are only three pairs of bonded electrons, leaving one unshared lone pair.

# Molecule with three bond pairs and one lone pair of electrons

- Lone pair bond pair repulsions change the angle from the tetrahedral angle to a slightly lower value of 107.5°.
- Typical molecules of this type are NH<sub>3</sub>, NF<sub>3</sub>, PCl<sub>3</sub>, etc



# Bent Molecules (i.e. those with two bond pairs and two lone pairs)

- A water molecule has a non-linear shape because it has two pairs of bonded electrons and two unshared lone pairs.
- The bond angle between the hydrogen atoms is 104.5° (away from the ideal tetrahedral angle of 109.5°)

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# Types of molecular structure relevant to organic chemistry

- **Bent:** The final basic shape of a molecule is the non-linear shape, also known as bent or angular.
- The four electron pairs (two bond pairs + two lone pairs) are distributed tetrahedrally around the central atom.
- The two lone pairs on the central atom repel the bond pair slightly inwards due to greater lone pair-bond pair repulsion.

# Summary of molecular shapes

Bonding Electron Pairs	Lone Pairs (on central atom)	Shape	Ideal Bond Angle (example's bond angle)	Example
2	0	linear	180°	CO <sub>2</sub>
3	0	Trignal	120°	BF <sub>3</sub>
4	0	Tetrahedral	109.5°	CH <sub>4</sub>
3	1	Trignal pyramidal	109.5° (107.5°)	NH <sub>3</sub>
2	2	Bent	109.5° (104.5°)	H <sub>2</sub> O
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# **Intermolecular Forces**

- The covalent bond holding a molecule together is an intramolecular force.
- The attraction between molecules is an intermolecular force.
- Intermolecular forces are much weaker than intramolecular forces (e.g. 16 kJ/mol vs. 431 kJ/mol for Hydrochloric acid, HCl).
- When a substance melts or boils the intermolecular forces are broken (not the covalent bonds).
- When a substance condenses intermolecular forces are formed.

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# Intermolecular forces

- As mentioned earlier, a polar molecule has a distorted electron cloud around the bond.
- The bond has a slightly positive end,  $\delta$ +, and a slightly negative end,  $\delta$ -.
- Such a molecule is known as a dipole.
- I.e. Dipole = a molecule (or part of a molecule) with a positive end and a negative end

# **Dipole-dipole interactions**

- All molecules (polar and non-polar) exert a weak attraction upon the other, due to the electrostatic attraction of the electrons of one molecule to the nuclei of the other.
- These forces are known as van der Waals forces.
- They occur in all kinds of molecular solids including non-polar molecules such as H<sub>2</sub>, O<sub>2</sub>, Cl<sub>2</sub>, CH<sub>4</sub>, etc. and are present in both solid and liquid states.

# **Types of Dipoles**

- Instantaneous dipole
- Induced Dipole
- Permanent Dipole

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# Instantaneous dipole

- Weak intermolecular forces that arise from the interactive forces between temporary multipoles in molecules without permanent multipole moments. In fact, they are much weaker than other types of intermolecular forces.
- Occur between <u>all</u> molecules.
- They are known as London dispersion forces, named after the German-American physicist Fritz London.

## Instantaneous dipole

 For example, halogens Fluorine and chlorine are gases at room temperature, bromine is a liquid, and iodine is a solid. The London forces also become stronger with larger amounts of surface contact. Greater surface area means closer interaction between different molecules

# Instantaneous dipole

- Without London forces, there would be no attractive force between noble gas atoms, and they wouldn't exist in liquid form.
- London forces become stronger as the atom or molecule in question becomes larger. This is due to the increased polarizability of molecules with larger, more dispersed electron clouds.

# Induced dipoles The permanent dipole of a molecule can induce a dipole in an unpolarised molecule. When a non-polar molecule approaches a polar molecule (with a permanent dipole), a dipole will be induced in the non-polar molecule. The dipole induced will be in opposite orientation to that of the polar molecule. The dipole induced will be in opposite orientation to that of the polar molecule.

HCI molecule with a permanent dipole

positive end of the HCl dipole - this induces a dipole in the Cl<sub>2</sub> molecule.

# **Permanent Dipoles**

- When a molecule has a dipole it is *polarised*
- These occur when a two atoms sharing a covalent bond have <u>substantially different</u> electronegativity.
- HCl has a permanent dipole as Cl has a much higher electronegativity than H.
- Molecules with a permanent dipole are polar molecules.

# Hydrogen bond

 A hydrogen bond is the attractive force between one electronegative atom and a hydrogen covalently bonded to another electronegative atom. It results from a dipoledipole force with a hydrogen atom bonded to nitrogen, oxygen or fluorine (thus the name "hydrogen bond", which must not be confused with a covalent bond to hydrogen).

# Hydrogen bond

- The energy of a hydrogen bond (typically 5 to 30 kJ/mole) is comparable to that of weak covalent bonds (155 kJ/mol), and a typical covalent bond is only 20 times stronger than an intermolecular hydrogen bond.
- These bonds can occur between molecules (*intermolecularly*), or within different parts of a single molecule (*intramolecularly*).

# Hydrogen bond

- The hydrogen bond is a very strong fixed dipole-dipole van der Waals, but weaker than covalent, ionic bonds.
- The hydrogen bond is somewhere between a covalent bond and an electrostatic intermolecular attraction.
- This type of bond occurs in both inorganic molecules (such as water) and organic molecules (such as DNA)

# Hydrogen bond

- Liquids that display hydrogen bonding are called **associated liquids**.
- Hydrogen bonds can vary in strength from very weak (1-2 kJ mol<sup>-1</sup>) to extremely strong (>155 kJ mol<sup>-1</sup>), as in the ion HF<sub>2</sub><sup>-</sup>.

# Hydrogen bond

- Liquid water's high boiling point is due to the high number of hydrogen bonds each molecule can have relative to its low molecular mass, not to mention the great strength of these hydrogen bonds.
- Realistically the water molecule has a very high boiling point, melting point and viscosity compared to other similar substances not conjoined by hydrogen bonds

# Hydrogen bond

- Typical values include:
  - F-H...:F (155 kJ/mol or 40 kcal/mol)
  - O-H.::N (29 kJ/mol or 6.9 kcal/mol)
  - -O-H.:O (21 kJ/mol or 5.0 kcal/mol)
  - N-H.: N (13 kJ/mol or 3.1 kcal/mol)
  - N-H.:: O (8 kJ/mol or 1.9 kcal/mol)
  - HO—H<sup>...</sup>:OH<sub>3</sub><sup>+</sup> (18 kJ/mol or 4.3 kcal/mol)

# Difference between hydrogen bond and covalent bond

Hydrogen Bond	Covalent Bond		
This bond involves dipole to dipole movement	This bond involves sharing of electrons		
It is formed between hydrogen	It is formed between any two		
atom and a higher electronegative	electronegative atoms, which may be		
atom (F, O or N)	of the same or different elements		
The bond strength of hydrogen is	Strength of covalent bonds is		
very small, e.g. HF bond is 41.83	sufficiently high, eg. H — H bond is		
kJmol <sup>-1</sup>	433 kJmol <sup>-1</sup>		

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