Course: Chemistry-II (6457)
Semester: Spring, 2021
Assignment No.1

Q.1 What is meant by a periodic table? Discuss the modern periodic table.

The First Periodic Table

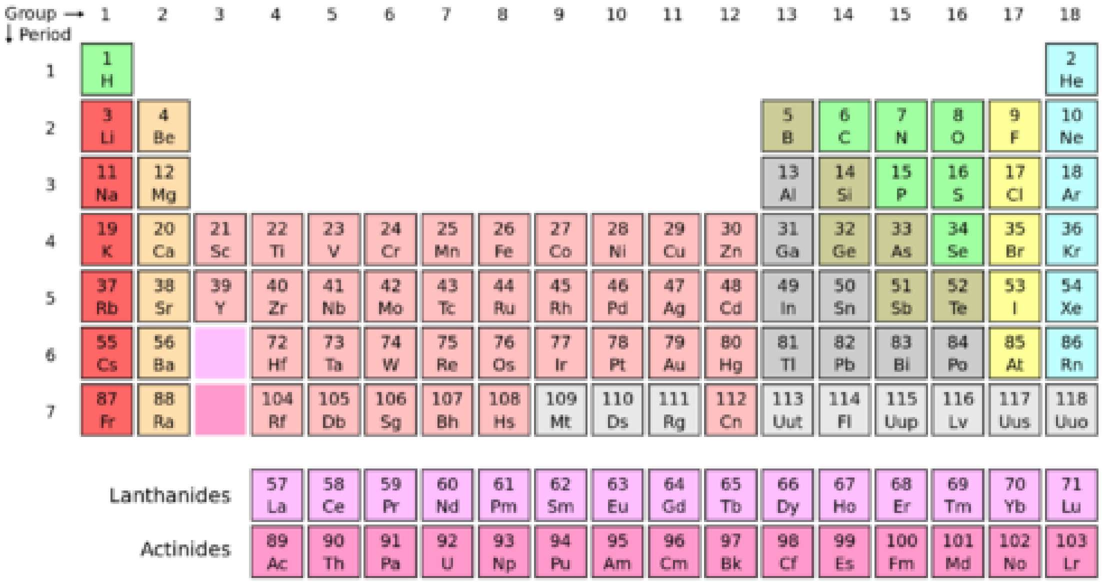
In the 1860s, a scientist named Dmitri Mendeleev also saw the need to organize the elements. He created a table in which he arranged all of the elements by increasing atomic mass from left to right across each row. When he placed eight elements in each row and then started again in the next row, each column of the table contained elements with similar properties. He called the columns of elements groups. Mendeleev's table is called a **periodic table** and the rows are called periods. That's because the table keeps repeating from row to row, and periodic means "repeating."

The Modern Periodic Table

A periodic table is still used today to organize the elements. You can see a simple version of the modern periodic table in the **Figure** below. The modern table is based on Mendeleev's table, except the modern table arranges the elements by increasing atomic number instead of atomic mass. Atomic number is the number of protons in an atom, and this number is unique for each element. The modern table has more elements than Mendeleev's table because many elements have been discovered since Mendeleev's time.

The periodic table has undergone extensive changes in the time since it was originally developed by Mendeleev and Moseley. Many new elements have been discovered, while others have been artificially synthesized. Each fits properly into a **group** of elements with similar properties. The periodic table is an arrangement of the elements in order of their atomic numbers so that elements with similar properties appear in the same vertical column or group.

The figure below shows the most commonly used form of the periodic table. Each square shows the chemical symbol of the element along with its name. Notice that several of the symbols seem to be unrelated to the name of the element: Fe for iron, Pb for lead, etc. Most of these are the elements that have been known since ancient times and have symbols based on their Latin names. The atomic number of each element is written above the symbol.



Group → ↓ Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
Lanthanides				57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinides				89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

A **period** is a horizontal row of the periodic table. There are seven periods in the periodic table, with each one beginning at the far left. A new period begins when a new principal energy level begins filling with electrons. Period 1 has only two elements (hydrogen and helium), while periods 2 and 3 have 8 elements. Periods 4 and 5 have 18 elements. Periods 6 and 7 have 32 elements because the two bottom rows that are separated from the rest of the table belong to those periods. They are pulled out in order to make the table itself fit more easily onto a single page.

A group is a vertical column of the periodic table, based on the organization of the outer shell electrons. There are a total of 18 groups. There are two different numbering systems that are commonly used to designate groups and you should be familiar with both. The traditional system used in the United States involves the use of the letters A and B. The first two groups are 1A and 2A, while the last six groups are 3A through 8A. The middle groups use B in their titles. Unfortunately, there was a slightly different system in place in Europe. To eliminate confusion the International Union of Pure and Applied Chemistry (IUPAC) decided that the official system for numbering groups would be a simple 1 through 18 from left to right. Many periodic tables show both systems simultaneously.

- **group:** Elements with similar chemical properties appear at regular intervals, within the vertical columns.
- **period:** A period is a horizontal row of the periodic table.

Classification of the Elements in the Periodic Table:

Classification of the elements in the periodic table can be done in four ways on the basis of their electronic configurations:

1. Noble gas elements:

Elements of group 18 of the modern periodic table are considered a noble gas. The electronic configuration of the first element (helium) of this group is 1s2. Rest all the elements (neon, argon, krypton, xenon, and radon) have their outer shell electronic configuration is ns2np6. As the octet of these elements is complete, hence they are highly stable elements.

2. Representative elements:

S-lock and P-block elements come under the category of representative elements. Elements in groups 1 and 2 are known as the s – block elements (elements with 1s2and 2s2 outermost configuration). Group 13-17 are known as the p-block elements (outermost configuration varies from ns2np1 to ns2np5).

3. Transition elements:

Elements which belong to group 3 to 12 and have their outer shell electronic configuration as (n-1)d1-10ns1-2 are referred to as transition elements. These elements are also known as the d-block elements.

4. Inner transition elements:

Lanthanides and actinides series which falls at the bottom of the periodic table comes under the category of inner transition elements. In these elements the 4f and 5f orbitals are partially filled, rendering them special properties.

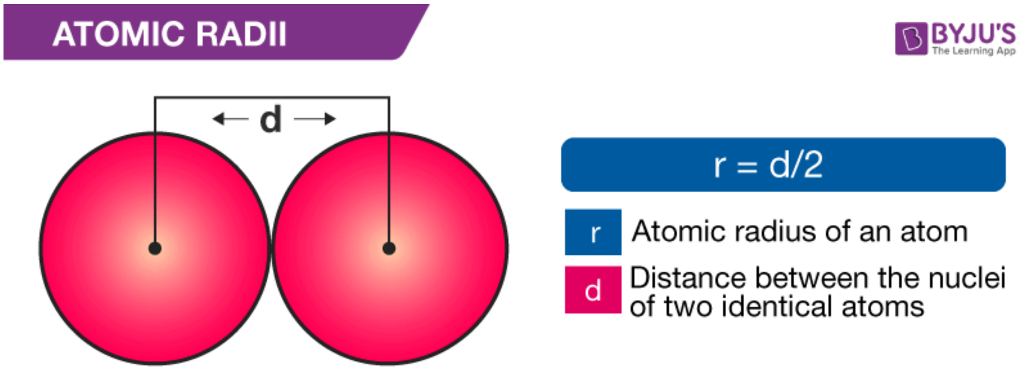
Q.2 Discuss the concept of atomic radius. How the covalent radii are differentiated from atomic radii?

Atomic radius is generally stated as being the total distance from an atom's nucleus to the outermost orbital of electron. In simpler terms, it can be defined as something similar to the radius of a circle, where the center of the circle is the nucleus and the outer edge of the circle is the outermost orbital of electron. As you begin to move across or down the periodic table, trends emerge that help explain how atomic radii change.

The effective nuclear charge (Zeff) of an atom is the net positive charge felt by the valence electron. Some positive charge is shielded by the core electrons therefore the total positive charge is not felt by the valence electron. A detailed description of shielding and effective nuclear charge can be found here. Zeff greatly affects the atomic size of an atom. So as the Zeff decreases, the atomic radius will grow as a result because there is more screening of the electrons from the nucleus, which decreases the attraction between the nucleus and the electron. Since Zeff decreases going down a group and right to left across the periodic table, the atomic radius will increase going down a group and right to left across the periodic table.

- An atom is made up of three tiny kinds of particles called subatomic particles: protons, neutrons, and electrons.
- The protons and the neutrons make up the center of the atom called the nucleus and the electrons fly around above the nucleus in a small cloud.
- The electrons carry a negative charge and the protons carry a positive charge.
- In a neutral atom the number of protons and the number of electrons are equal. Often, but not always, the number of neutrons is the same, too.
- The radius of a circle is the distance from the centre point to the edge of the circle.

- It’s the same distance anywhere on the circle because the circle has radial symmetry.



Atomic radius or Atomic Radii is the total distance from the nucleus of an atom to the outermost orbital of its electron. We can define the atomic radius of a chemical element as:

The measure of the size of its atoms, usually the mean or typical distance from the center of the nucleus to the boundary of the surrounding shells of electrons.

- This is mostly similar to the idea of the radius of a circle, where we can consider the nucleus to be the centre of the circle and the outermost orbital of the electron to be the outer edge of the circle.
- It is really difficult to determine the atomic radii because of the uncertainty in the position of the outermost electron. We can not say the exact position of the electron.
- Heisenberg Uncertainty Principle can be used to get a precise measurement of the radius but again it is not a completely correct one.
- As per the principle, we determine the radius based on the distance between the nuclei of two bonded atoms. The radii of atoms are therefore determined by the bonds they form. An atom will have different radii depending on the bond it forms; so there is no fixed radius of an atom.
- The different radius is van der Waals radius, ionic radius, metallic radius and covalent radius.

Types of Radius with Respect to the Types of Bonds

1. Van Der Waals Radius:

Van-der-Waals radii are determined from the contact distances between unbonded atoms in touching molecules or atoms.

2. Ionic Radius:

- The ionic radius is the radius of an atom forming an ionic bond or an ion.
- The electrons and nucleus are restricted by the atomic bonds and due to this reason the ions or atoms don’t have a specific shape.
- The measuring unit for the ionic radius is Armstrong(A0) or picometers(pm). The characteristic radius ranges from 30 to 200 pm.
- The ionic radius is not static but differs with respect to spin state of the electrons, coordination number and numerous other parameters.

- Ionic size grows with increasing coordination number. The ionic size also grows for an ion with the high spin state of an electron than an ion with a low spin state of the electron.
- The ion with a positive charge will have a smaller size than the ion with negative charge if we will take charge of the ion into consideration.

3. Metallic Radius:

The metallic radius is the radius of an atom joined by the metallic bond. The metallic radius is half of the total distance between the nuclei of two adjacent atoms in a metallic cluster.

4. Covalent Radius:

- The covalent radius of an atom is stated as the radius of an atom which is under the covalent bond with another atom(s) of a similar element.
- The covalent radius of an atom can be determined by measuring bond lengths between pairs of covalently-bonded atoms: if the two atoms are of the same kind, then the covalent radius is simply one half of the bond length.
- Whilst this is straightforward for some molecules such as Cl2 and O2, in other cases, one has to infer the covalent radius by measuring bond distances to atoms whose radii are already known (e.g., a C–X bond, in which the radius of C is known).

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Q.3 Explain the molecular interactions. Discuss the nature chemical bonds.

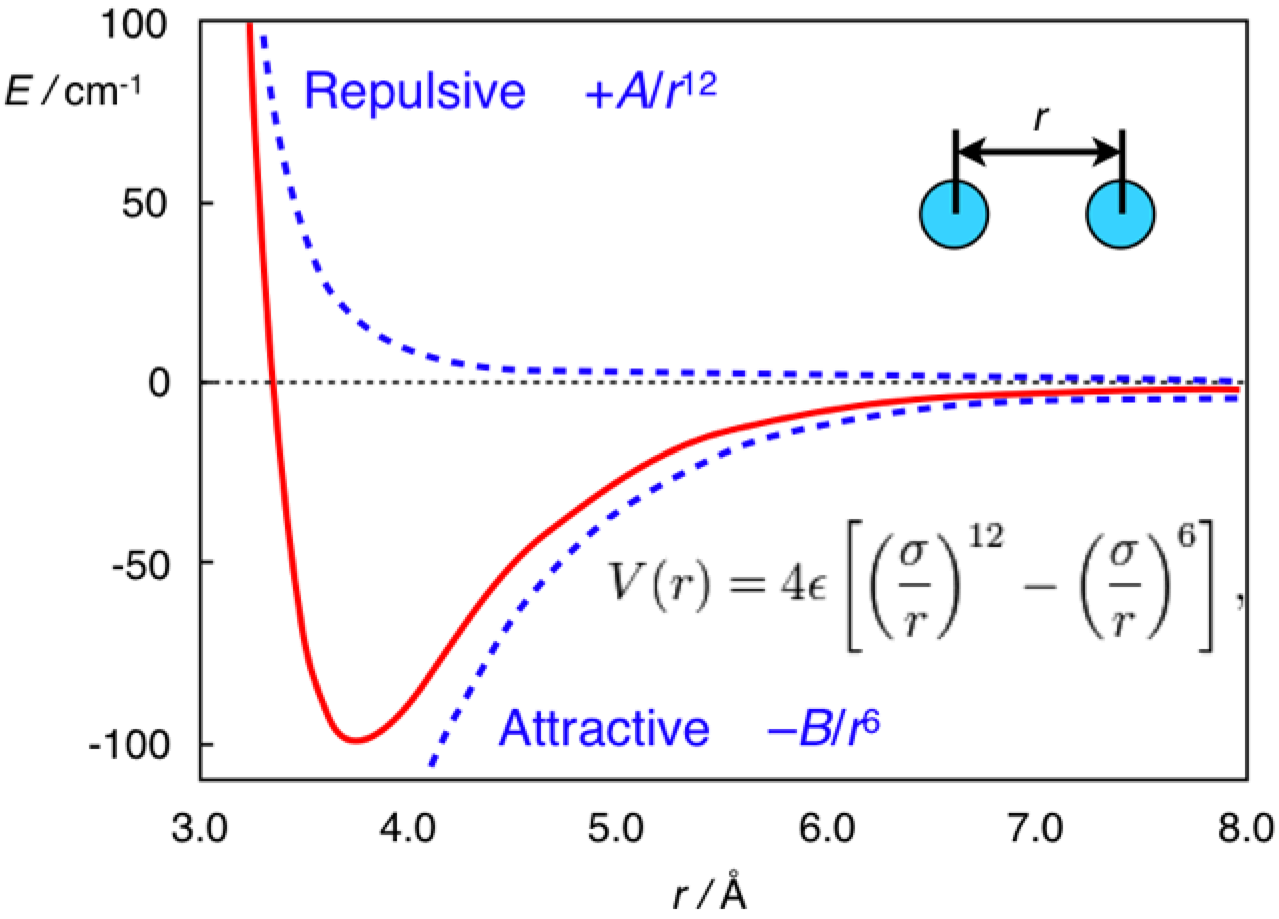
Much of medicinal chemistry is based on the optimisation or reduction of interactions between a small molecule and a variety of biomolecules, this can be increasing the affinity of a ligand for a receptor or reducing affinity for some undesired off-target interaction such as HERG or CYP450. Whilst the overall physicochemical properties of the molecule can have a major influence it likely that specificity might be driven by optimisation of strength and geometry of specific molecular interactions.

Strength of interactions

Whilst the strength of a covalent single bond is usually in the region 80-100 Kcal/mol the non-covalent interactions exploited by medicinal chemists are much weaker. Andrews has tried to estimate the average strength of various molecular interactions by examining the structural components and binding affinities of 200 compounds. Other have tried to estimate the strength of interaction by using chemical double mutants.

Typical Energies Salt Bridge ~2 kcal/mol H-Bond ~1 kcal/mol Hydrophobic ~0.7 kcal/mol Aromatic ~1-3 kcal/mol

Since dG=-2.303RTlogK we can calculate that a single ionic interaction might afford a 25-fold increase in affinity, whilst a hydrogen bond yield a 6-fold increase, 3.5-fold increase in binding constant for a methyl group. However it is important to note that steric clashes can have a much more pronounced impact on affinity, the interaction between two atoms is described by the Lennard-Jones potential shown graphically below.



As you can see the attractive forces predominate when the atoms are further apart but when they get too close the repulsive forces become dramatically dominant. Hence a small steric clash can cause the loss of all affinity.

Specific Interactions

With many of these interactions simply looking at a model of a protein with a ligand docked can be misleading, only considering the bound state only gives part of the equation. Desolvation plays a very important role, particularly with ionised or polar functional groups where there will be a large unfavourable desolvation term, in addition entropic changes can also have a significant influence.

A detailed analysis of the molecular interactions present found between ligands and macromolecules has been undertaken, "A systematic analysis of atomic protein–ligand interactions in the PDB" DOI looking at over 11,000 complexes the authors were able to categorise the 7 most common types of interaction Fig 1. (Image curtesy of Matthieu Schapira).

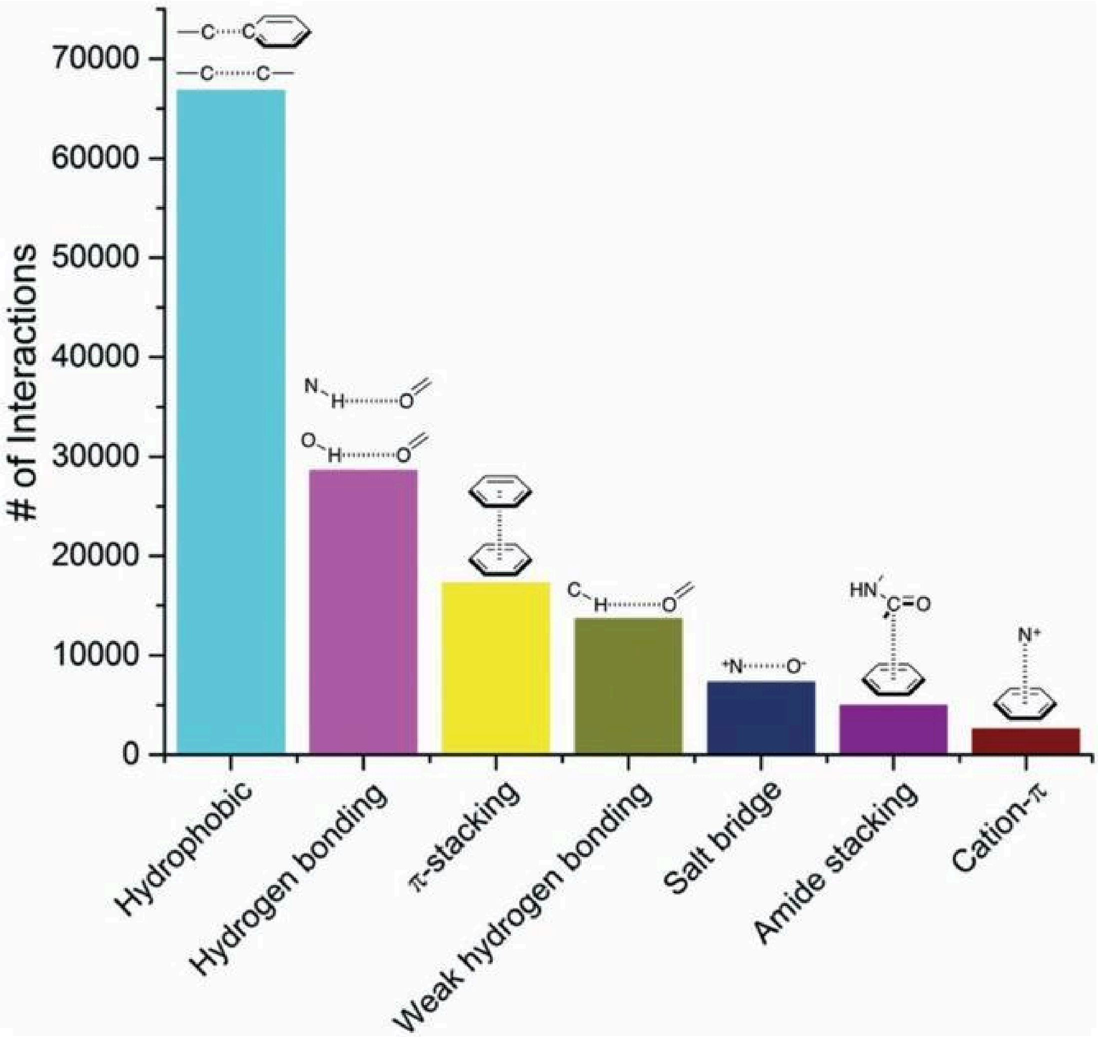
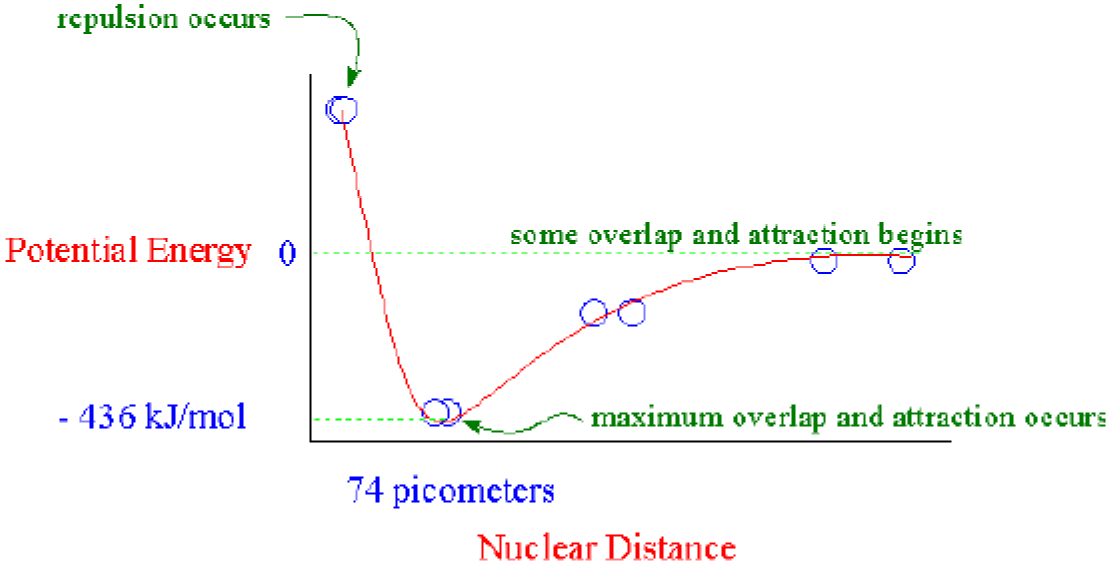


Fig. 1 Frequency distribution of the most common non-covalent interactions observed in protein–ligands extracted from the PDB.

Chemical bonds are the attractive forces that hold atoms together in the form of compounds. They are formed when electrons are shared between two atoms. There are 3 types of bonds: covalent bonds, polar covalent bonds and ionic bonds. The simplest example of bonding can be demonstrated by the H_2 molecule. We can see from the periodic table that each hydrogen atom has a single electron. If 2 hydrogen atoms come together to form a bond, then each hydrogen atom effectively has a share in both electrons and thus each resembles a noble gas and is more stable. The 2 electrons that are shared can be represented either by 2 dots or a single dash between the atoms.

$$\mathrm{H}\cdot \quad + \quad \cdot\mathrm{H} \longrightarrow \mathrm{H}:\mathrm{H} \quad \text{or} \quad \mathrm{H}-\mathrm{H}$$

Valence bond theory describes a chemical bond as the overlap of atomic orbitals. In the case of the hydrogen molecule, the 1s orbital of one hydrogen atom overlaps with the 1s orbital of the second hydrogen atom to form a molecular orbital called a sigma bond. Attraction increases as the distance between the atoms gets closer but nuclear-nuclear repulsion becomes important if the atoms approach too close.



There are 3 methods of showing the formulas of molecules. Molecular formulas show only the types and numbers of atoms in the molecule. Structural formulas show the atoms in their correct placement in the molecule and allow for distinguishing isomers. Electron-dot formulas are similar to structural formulas but also include all of the non-bonding outer electrons. Knowledge of electron placement allows us to understand not only the shape of molecules but their chemical character. If we understand the chemical character of a molecule, we can predict how it will react with other molecules without having to blindly memorize reactions.

Q.4 Discuss the formation and characteristics of an Ionic Bond.

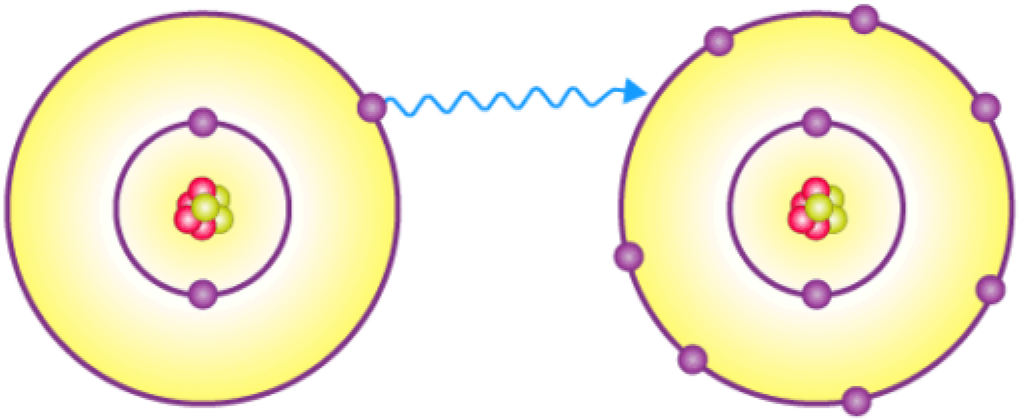
The electrostatic force of attraction which holds the two oppositely charged ions together is called the ionic bond.

A chemical bond is formed between two atoms by the complete transfer of one or more electrons from one atom to the other as a result of which the atoms attain their nearest inert gas configuration.

There are primarily three ways in which two atoms combine to lose energy and to become stable. One of the ways is by donating or accepting electrons to complete their octet configuration. The bond formed by this kind of combination is known as an **ionic bond** or **electrovalent bond**. This kind of bond is formed when one atom gains electrons while the other atom loses electrons from its outermost level or orbit.

Electrovalent Bond

Electrovalent bonds are produced when electrons are transferred from atoms of one element to atoms of another element, producing positive and negative ions. The bond which is formed by the transfer of electrons between the atoms is called electrovalent bond or ionic bond. Electrovalent bonds are only formed between metals and non-metals. Electrovalent bonds are not formed between two non-metals.



Ionic Bond (Electrovalent Bond)

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In simple words electrovalent bond involves the transference of a certain number of electrons to another dissimilar atom which has a tendency to gain electrons so that both acquire stable inert gas configurations. The electrostatic attraction always tends to decrease the potential energy. Hence, the potential energy of the system is much less than it was before the formation of an ionic bond.

Electronegativity and Ionic Bonding

- An Ionic bond is the bond formed by the complete transfer of valence electron to attain stability.
- This type of bonding leads to the formation of two oppositely charged ions – positive ion known as **cations** and negative ions are known as **anions**.
- The presence of two oppositely charged ions results in a strong attractive force between them. This force is an ionic or electrovalent bond.
- Ionic bonds form between atoms with large differences in electronegativity, whereas covalent bonds formed between atoms with smaller differences in electronegativity.
- The compound formed by the electrostatic attraction of positive and negative ions is called an ionic compound.

Ionic Bond Vs Covalent Bond

Ionic Bond	**Covalent Bond**
The ionic bond is the attraction between positive and negative ions in a crystal and compounds held together by ionic bonds are called ionic compounds.	The covalent bond is a bond formed when two atoms share one or more electron pairs. Each atom contributes an equal number of electrons towards the bond formation.

If the difference of ionization potential between the two atoms is more ionic compounds are formed.	Atoms with higher ionization potential are unable to lose their valence electrons and hence prefer to form covalent bonds by sharing of electrons.
Atoms with greater electronegativity difference lead to the formation of an ionic bond.	If the electronegativities of the combining atoms do not differ much then the bond formed between them is likely to be covalent.
Example: NaCl	Example: HCl

Ionic Bond Properties

Due to the presence of a strong force of attraction between cations and anions in ionic bonded molecules, the following properties are observed:

1. The ionic bonds are the strongest of all the bonds.
2. The ionic bond has charge separation, and so they are the most reactive of all the bonds in the proper medium.
3. The ionic bonded molecules have high melting and boiling point.
4. The ionic bonded molecules in their aqueous solutions or in the molten state are good conductors of electricity. This is due to the presence of ions which acts as charge carriers.

Examples of Ionic Bonds

The following table shows the elements and the ions formed by them when they lose or gain e.

Element	**Electronic config.**	**Reaction**	**Formed ion**
Na(11)	2,8,1	$Na \rightarrow Na^+ + e^-$ ………………….. Reaction 1	Na^+
Ca(20)	2,8,8,2	$Ca \rightarrow Ca^{2+} + 2e^-$……………….. Reaction 2	Ca^{2+}
Cl(17)	2,8,7	$Cl + e^- \rightarrow Cl^-$ ···…………….……. Reaction 3	Cl^-
O(8)	2,6	$O + 2e^- \rightarrow O^{2-}$…………………… Reaction 4	O^{2-}

- Now when Na reacts with Cl, reaction 1 and reaction 3 will take place and the resultant compound will be NaCl.
- When Na reacts with O, reaction 1 and reaction 4 will take place and the resultant compound will be Na_2
- When Ca reacts with Cl, reaction 2 and reaction 3 will take place and the resultant compound will be $CaCl_2$.

- When Ca reacts with O, reaction 2 and reaction 4 will take place and the resultant compound will be CaO.

Q.5 Elaborate the Valence Bond Theory (VBT). How it helps to determine the shape of molecules?

Many approaches have been put forth to explain the nature of bonding in coordination compounds. One of them is the Valence Bond (VB) Theory. The Valence Bond Theory was developed in order to explain chemical bonding using the method of quantum mechanics. This theory primarily focuses on the formation of individual bonds from the atomic orbitals of the participating atoms during the formation of a molecule.

According to the valence bond theory,

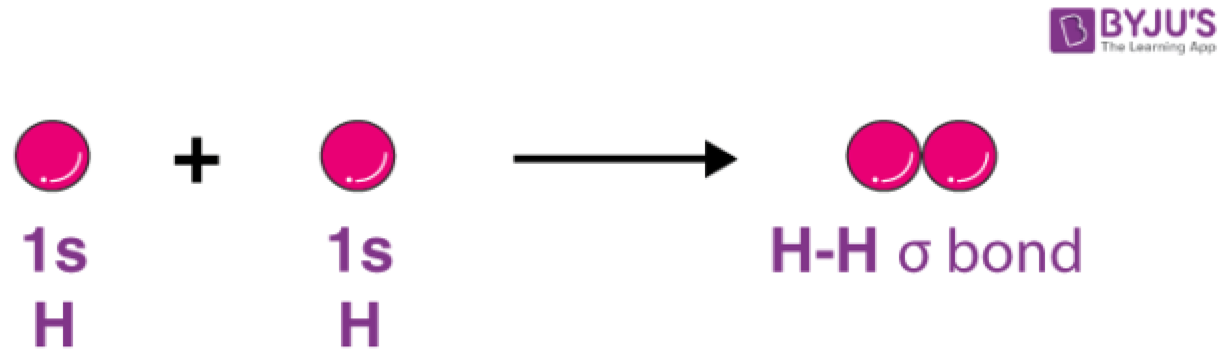
Electrons in a molecule occupy atomic orbitals rather than molecular orbitals. The atomic orbitals overlap on the bond formation and the larger the overlap the stronger the bond.

The metal bonding is essentially covalent in origin and metallic structure involves resonance of electron-pair bonds between each atom and its neighbors.

History of Valence Bond Theory

The Lewis approach to chemical bonding failed to shed light on the formation of chemical bonds. Also, valence shell electron pair repulsion theory (or VSEPR theory) had limited applications (and also failed in predicting the geometry corresponding to complex molecules).

In order to address these issues, the valence bond theory was put forth by the German physicists Walter Heinrich Heitler and Fritz Wolfgang London. The Schrodinger wave equation was also used to explain the formation of a covalent bond between two hydrogen atoms. The chemical bonding of two hydrogen atoms as per the valence bond theory is illustrated below.



This theory focuses on the concepts of electronic configuration, atomic orbitals (and their overlapping) and the hybridization of these atomic orbitals. Chemical bonds are formed from the overlapping of atomic orbitals wherein the electrons are localized in the corresponding bond region.

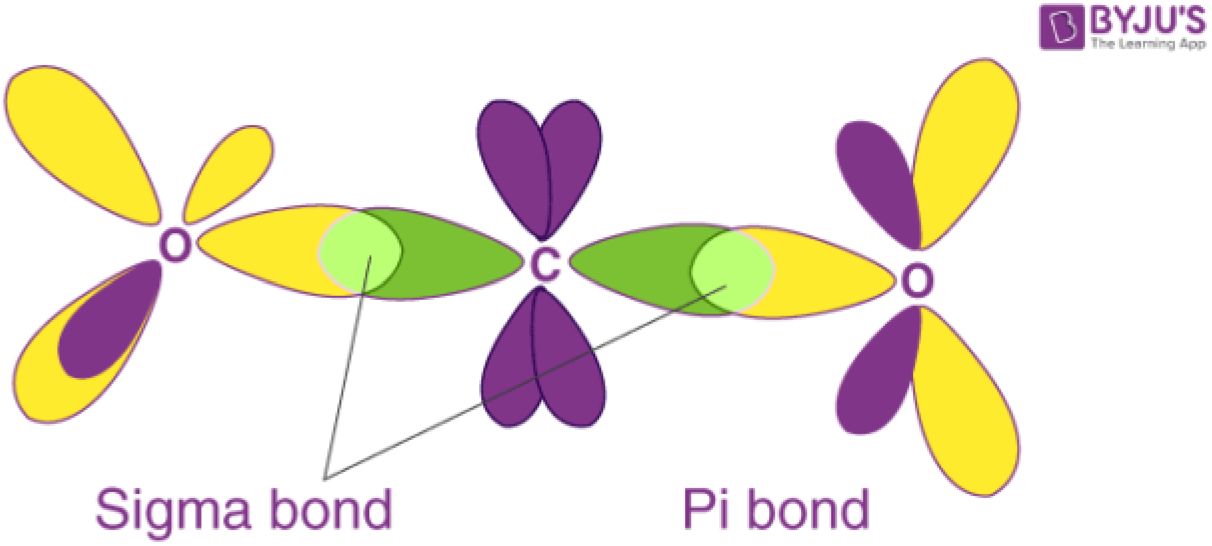
The valence bond theory also goes on to explain the electronic structure of the molecules formed by this overlapping of atomic orbitals. It also emphasizes that the nucleus of one atom in a molecule is attracted to the electrons of the other atoms.

Postulates of Valence Bond Theory

The important postulates of the valence bond theory are listed below.

1. Covalent bonds are formed when two valence orbitals (half-filled) belonging to two different atoms overlap on each other. The electron density in the area between the two bonding atoms increases as a result of this overlapping, thereby increasing the stability of the resulting molecule.
2. The presence of many unpaired electrons in the valence shell of an atom enables it to form multiple bonds with other atoms. The paired electrons present in the valence shell do not take participate in the formation of chemical bonds as per the valence bond theory.
3. Covalent chemical bonds are directional and are also parallel to the region corresponding to the atomic orbitals that are overlapping.
4. Sigma bonds and pi bonds differ in the pattern that the atomic orbitals overlap in, i.e. pi bonds are formed from sidewise overlapping whereas the overlapping along the axis containing the nuclei of the two atoms leads to the formation of sigma bonds.

The formation of sigma and pi bonds is illustrated below.



Formation of Sigma and Pi Bonds – Valence Bond Theory (VBT)

It can be noted that sigma bonds involve the head-to-head overlapping of atomic orbitals whereas pi bonds involve parallel overlapping.

Number of Orbitals and Types of Hybridization

According to VBT theory the metal atom or ion under the influence of ligands can use its (n-1)d, ns, np, or ns, np, nd orbitals for hybridization to yield a set of equivalent orbitals of definite geometry such as octahedral, tetrahedral, square planar and so on. These hybrid orbitals are allowed to overlap with ligand orbitals that can donate electron pairs for bonding.

Coordination Number	**Type of Hybridisation**	**Distribution of Hybrid Orbitals in Space**
4	sp^3	Tetrahedral
4	dsp^2	Square planar
5	sp^3d	Trigonal bipyramidal
6	sp^3d^2	Octahedral
6	d^2sp^3	Octahedral

Applications of Valence Bond Theory

- The maximum overlap condition which is described by the valence bond theory can explain the formation of covalent bonds in several molecules.
- This is one of its most important applications. For example, the difference in the length and strength of the chemical bonds in H_2 and F_2 molecules can be explained by the difference in the overlapping orbitals in these molecules.
- The covalent bond in an HF molecule is formed from the overlap of the 1s orbital of the hydrogen atom and a 2p orbital belonging to the fluorine atom, which is explained by the valence bond theory.

Limitations of Valence Bond Theory

The shortcomings of the valence bond theory include

- Failure to explain the tetravalency exhibited by carbon.
- No insight offered on the energies of the electrons.
- The theory assumes that electrons are localized in specific areas.
- It does not give a quantitative interpretation of the thermodynamic or kinetic stabilities of coordination compounds.
- No distinction between weak and strong ligands.
- No explanation for the colour exhibited by coordination compounds.