L.S COLLEGE MUZAFFARPUR

B. R. A. BIHAR UNIVERSITY

Dr Kalpna Kumari

Department of Chemistry

L.S. College Muzaffarpur

TOPIC :- CHEMICAL BONDING

What is Chemical Bonding?

Chemical Bonding refers to the formation of a chemical bond between two or more atoms, molecules, or ions to give rise to a chemical compound. These chemical bonds are what keep the atoms together in the resulting compound.

The attractive force which holds various constituents (atom, ions, etc.) together and stabilizes them by the overall loss of energy is known as chemical bonding. Therefore, it can be understood that chemical compounds are reliant on the strength of the chemical bonds between its constituents; The stronger the bonding between the constituents, the more stable the resulting compound would be.

The opposite also holds true; if the chemical bonding between the constituents is weak, the resulting compound would lack stability and would easily undergo another reaction to give a more stable chemical compound (containing stronger bonds). To find stability, the atoms try to lose their energy.

Whenever matter interacts with another form of matter, a force is exerted on one by the other. When the forces are attractive in nature, the energy decreases. When the forces are repulsive in nature, the energy increases. The attractive force that binds two atoms together is known as the chemical bond.

Important Theories on Chemical Bonding

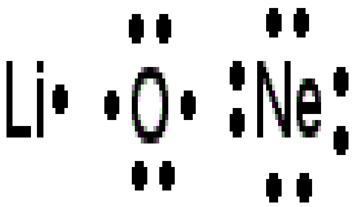
Albrecht Kössel and Gilbert Lewis were the first to explain the formation of chemical bonds successfully in the year 1916. They explained chemical bonding on the basis of the inertness of noble gases.

Lewis Theory of Chemical Bonding

- An atom can be viewed as a positively charged 'Kernel' (the nucleus plus the inner electrons) and the outer shell.
- The outer shell can accommodate a maximum of eight electrons only.
- The eight electrons present in the outer shell occupy the corners of a cube which surround the 'Kernel'.

- The atoms having octet configuration, i.e. 8 electrons in the outermost shell, thus symbolize a stable configuration.
- Atoms can achieve this stable configuration by forming chemical bonds with other atoms. This chemical bond can be formed either by gaining or losing an electron(s) (NaCl, MgCl2) or in some cases due to the sharing of an electron (F2).
- Only the electrons present in the outer shell, also known as the valence electrons take part in the formation of chemical bonds. Gilbert Lewis used specific notations better known as Lewis symbols to represent these valence electrons.
- Generally, the valency of an element is either equal to the number of dots in the corresponding Lewis symbol or 8 minus the number of dots (or valence electrons).

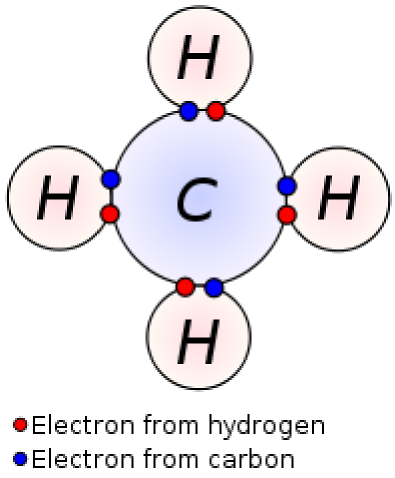
Lewis symbols for lithium (1 electron), oxygen (6 electrons), neon (8 electrons) are given below:



Here, the number of dots that surround the respective symbol represents the number of valence electrons in that atom.

Covalent Bonding

A covalent bond indicates the sharing of electrons between atoms. Compounds that contain carbon (also called organic compounds) commonly exhibit this type of chemical bonding. The pair of electrons which are shared by the two atoms now extend around the nuclei of atoms, leading to the creation of a molecule.



Covalent Bonding

Polar Covalent Bonding

Covalent bonds can be either be Polar or Non-Polar in nature. In Polar Covalent chemical bonding, electrons are shared unequally since the more electronegative atom pulls the electron pair closer to itself and away from the less electronegative atom. Water is an example of such a polar molecule.

A difference in charge arises in different areas of the atom due to the uneven spacing of the electrons between the atoms. One end of the molecule tends to be partially positively charged and the other end tends to be partially negatively charged.

Writing Lewis Structures

The following steps are adopted for writing the Lewis dot structures or Lewis structures:

Step 1: Calculate the number of electrons required for drawing the structure by adding the valence electrons of the combining atoms. **For Example**, in methane, CH_4 molecule, there are 8 valence electrons (in which 4 belongs to carbon while other 4 to H atoms).

Step 2: Each negative charge i.e. for anions, we add an electron to the valence electrons and for each positive charge i.e. for cations we subtract one electron from the valence electrons.

Step 3: Using the chemical symbols of the combining atoms and constructing a skeletal structure of the compound, divide the total number of electrons as bonding shared pairs between the atoms in proportion to the total bonds.

Step 4: The central position in the molecule is occupied by the least electronegative atom. Hydrogen and fluorine generally occupy the terminal positions.

Step 5: After distributing the shared pairs of electrons for single bonds, the remaining electron pairs are used for multiple bonds or they constitute lone pairs.

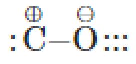
The basic requirement is that each bonded atom gets an octet of electrons.

Example 1: Lewis formula for carbon monoxide, CO

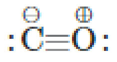
Step 1: Counting the total number of valence electrons of carbon and oxygen atoms: C ($2s^2 2p^2$) + O ($2s^2 2p^4$) 4 + 6 = 10 that is, 4(C) + 6(O) = 10

Step 2: The skeletal structure of carbon monoxide is written as CO

Step 3: Drawing a single bond between C and O and completing octet on O, the remaining two electrons are lone pair on C.



Step 4: This does not complete the octet of carbon, and hence we have a triple bond.



Example 2: Lewis Structure of nitrite, NO_2^-

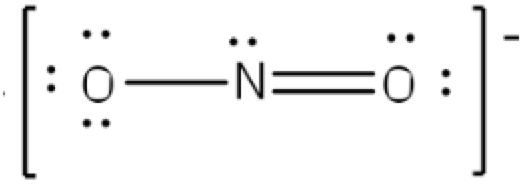
Step 1: Counting the total number of valence electrons of one nitrogen atom, two oxygen atoms and the additional one negative charge (equal to one electron). Total Number of valence electrons is: N ($2s^2 2p^3$) + 2O ($2s^2 2p^4$) + 1 (negative charge) => 5+ 2(6) +1=18e^-

Step 2: The skeletal structure of nitrite ion is written as O-N-O

Step 3: Drawing a single bond between nitrogen and each oxygen atom: O – N – O

Step 4: Complete the octets of atoms.

This structure does not complete octet on N if the remaining two electrons constitute of a lone pair on it. Therefore, we have a double bond between one N and one of the two O atoms. The Lewis structure is



What is Valance Bond (VB) Theory?

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.

Formation of Sigma Bonds between Two Atoms – Valence Bond Theory (VBT)

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.

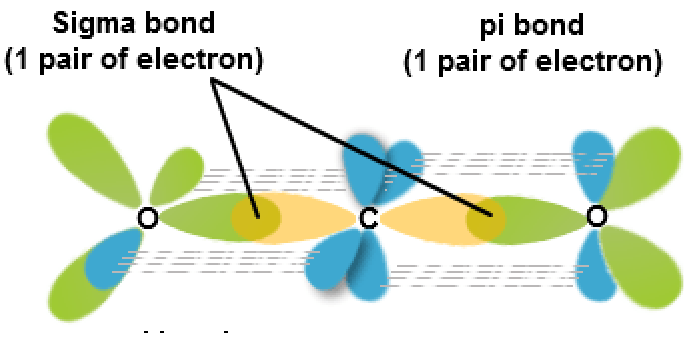
The valence bond theory also goes on to explain the electronic structure of the molecules formed by this overlapping of atomic orbitals. It also emphasizes that the nucleus of one atom in a molecule is attracted to the electrons of the other atoms.

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.