

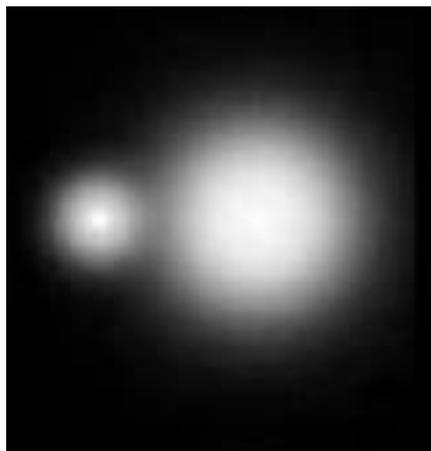
CHEMICAL BONDING

CLASSIFICATION AND TYPES
VALENCE BOND THEORY
MOLECULAR ORBITAL
THEORY

- Chemical compounds are formed by the bonding of two or more atoms. A stable bonding forms when the total energy of the combination has lower energy than the separated atoms. The bound state implies a net attractive force between the atoms called a chemical bond. Chemical bonds are classified in to many types.
- **Covalent bond:** bond in which one or more pairs of electrons are shared by two atoms.
- **Ionic bond:** bond in which one or more electrons from one atom are removed and attached to another atom, resulting in positive and negative ions which attract each other.
- Other types of bonds include **metallic bonds** and **hydrogen bonding**. The attractive forces between molecules in a liquid can be characterized as **Vanderwaals bonds**.

Ionic Bond Representation

NaCl–Ionic bond



Valence Bond Theory

- 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
- **Orbital hybridization** : The mixing of atomic orbitals to form new orbitals of suitable energy for chemical bonding

Types of Hybridization and Molecular Shapes

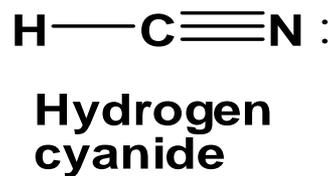
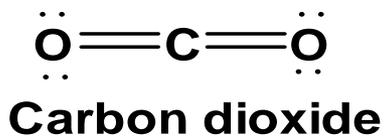
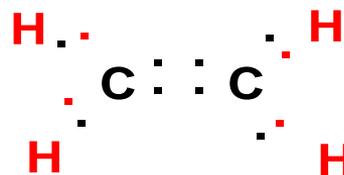
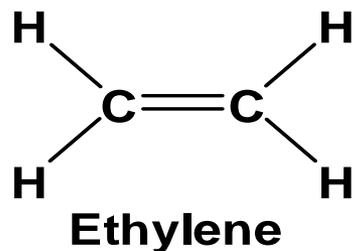
- sp^3 hybrids- Tetrahedral shape- e.g., CCl_4 , NH_3
- sp^2 hybrids- Trigonal planar shape- e.g., BCl_3
- sp hybrids- linear or diagonal- e.g., BeCl_2
- sp^3d hybrids- trigonal bipyramidal shape- e.g., PCl_5
- sp^3d^2 hybridisation; octahedral (or square bipyramidal) shape- e.g., SF_6

Hybridization of Carbon

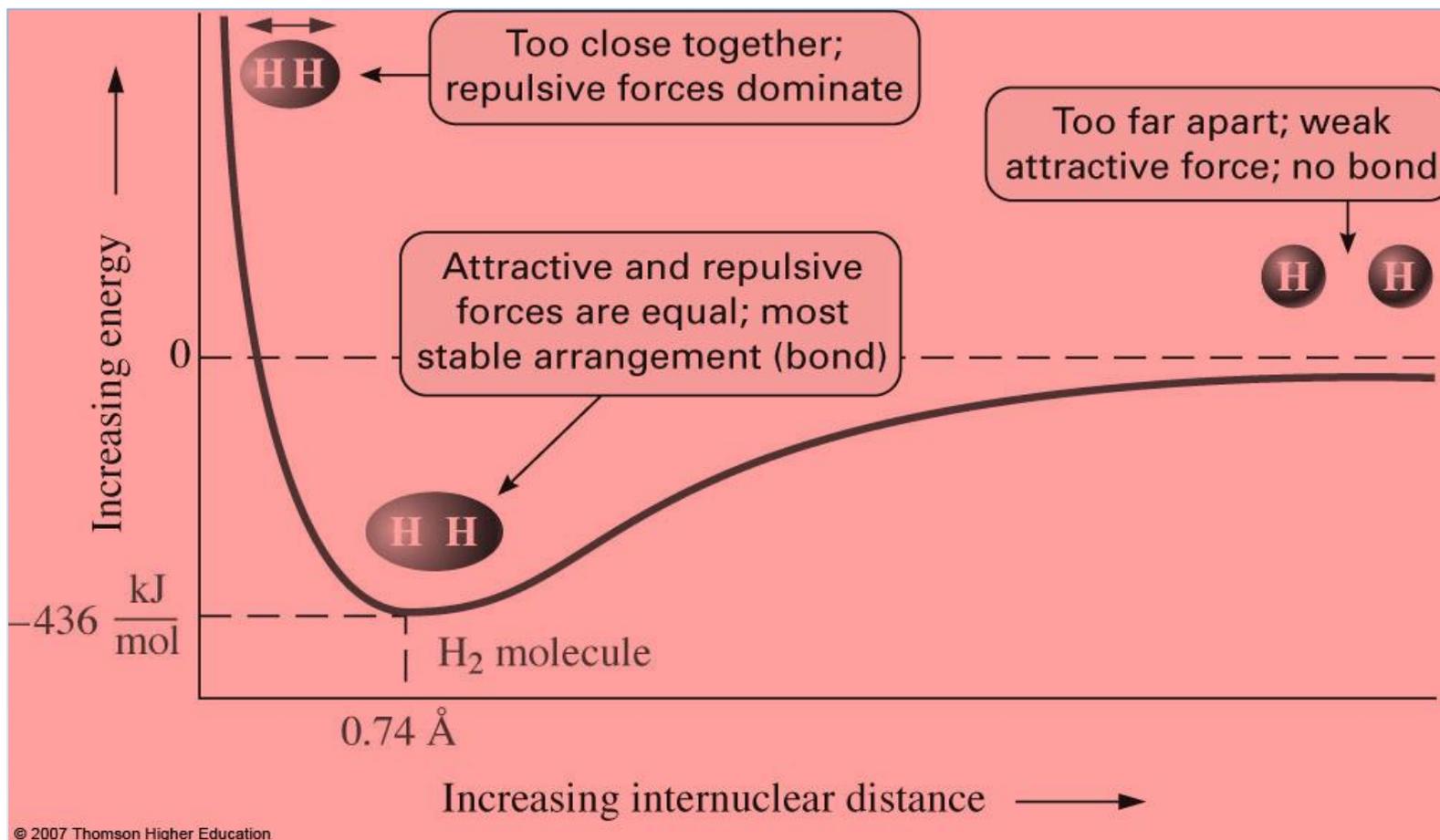
- The element, carbon forms virtually an infinite number of compounds. This is largely due to the types of bonds it can form and the number of different elements it can join in bonding. Carbon may form single, double and triple bonds. The hybridization of carbon involved in each of these bonds is illustrated as follows
- Bonding in any element will take place with only the valence shell electrons. The valence shell electrons are found in the incomplete, outermost shell. By looking at the electronic configuration, one can identify these valence electrons. Let's look at the electron configuration of ground state (lowest energy state) carbon which has 2 electrons in the 2s orbital and 2 electrons in the 2p orbital ($2p_x^1$ and $2p_y^1$) leaving a $2p_z$ orbital vacant

- **The 1s electrons are considered to be core electrons and are not available for bonding. There are two unpaired electrons in the 2p subshell, so if carbon were to hybridize from this ground state, it would be able to form at most two bonds. Recall that energy is released when bonds form, so it would be to carbon's benefit to try to maximize the number of bonds it can form. For this reason, carbon will form an excited state by promoting one of its 2s electrons into its empty 2p orbital and hybridize from the excited state. By forming this excited state, carbon will be able to form four bonds (sp^3 hybridization)**
- **The 2s and the 2p subshells are half-filled, so the excited state is relatively stable**

Lewis Formulas for Molecules and Polyatomic Ions



The Potential energy of H₂ as a function of The Distance Between the Two Nuclei



The valence bond (VB) approach to covalent bonding is basically concerned with the energetics of covalent bond formation about which the Lewis and VSEPR models are silent. Basically the VB theory discusses bond formation in terms of overlap of orbitals. For example the formation of the H₂ molecule from two hydrogen atoms involves the overlap of the 1s orbitals of the two H atoms which are singly occupied. It is seen that the potential energy of the system gets lowered as the two H atoms come near to each other.

At the equilibrium inter-nuclear distance (bond distance) the energy touches a minimum. Any attempt to bring the nuclei still closer results in a sudden increase in energy and consequent destabilization of the molecule. Because of orbital overlap the electron density between the nuclei increases which helps in bringing them closer. It is however seen that the actual bond enthalpy and bond length values are not obtained by overlap alone and other variables have to be taken into account.

For explaining the characteristic shapes of polyatomic molecules Pauling introduced the concept of **hybridisation of atomic orbitals**. *sp, sp², sp³ hybridizations of atomic orbitals* of Be, B, C, N and O are used to explain the formation and geometrical shapes of molecules like BeCl₂, BCl₃, CH₄, NH₃ and H₂O. They also explain the formation of multiple bonds in molecules like C₂H₂ and C₂H₄.

The **VSEPR model** used for predicting the geometrical shapes of molecules is based on the assumption that electron pairs repel each other and, therefore, tend to remain as far apart as possible. according to this model, molecular geometry is determined by repulsions between lone pairs and lone pairs ; lone pairs and bonding pairs and bonding pairs and bonding pairs. The order of these repulsions being :
 $lp-lp > lp-bp > bp-bp$

The **molecular orbital (MO) theory** describes bonding in terms of the combination and arrangement of atomic orbitals to form molecular orbitals that are associated with the molecule as a whole. The number of molecular orbitals are always equal to the number of atomic orbitals from which they are formed. Bonding molecular orbitals increase electron density between the nuclei and are lower in energy than the individual atomic orbitals.

Anti bonding molecular orbitals have a region of zero electron density between the nuclei and have more energy than the individual atomic orbitals. The electronic configuration of the molecules is written by filling electrons in the molecular orbitals in the order of increasing energy levels. As in the case of atoms, the Pauli exclusion principle and Hund's rule are applicable for the filling of molecular orbitals. Molecules are said to be stable if the number of electrons in bonding molecular orbitals is greater than that in anti bonding molecular orbitals.

ATOMIC STRUCTURE

AND

CHEMICAL BONDING

BOND ORDER

- $B.O = 1/2 (n - n^*)$
- n - No of electrons in the B.O.
- n^* - No of electrons in the Anti-B.O

Stern Gerlach Experiment

- SPIN OF ELECTRONS
- SILVER ATOMIC BEAM
- STRONG MAGNETIC FIELD
- Ag – At No: 47 ($23+23 = 46$ electrons spin paired)
- Remaining one electron unpaired. If it possesses same spin there will not be any splitting of the initial beam of atoms. But splitting into two beams observed because of the unpaired electron's spin in either direction