

Get Ready to Crack CSIR-NET 2021

(Short Notes on structure and
bonding in homo and
heteronuclear diatomic
molecules)



Structure and Bonding in homo and heteronuclear diatomic molecules

Diatomic molecules have only two atoms, which might be from the same or distinct chemical elements. Hydrogen (H_2), nitrogen (N_2), oxygen (O_2), and carbon monoxide (CO) are all common diatomic molecules (CO). At room temperature, seven elements exist as homonuclear diatomic molecules: H_2 , N_2 , O_2 , F_2 , Cl_2 , Br_2 , and I_2 .

Characteristics of Diatomic Molecule :

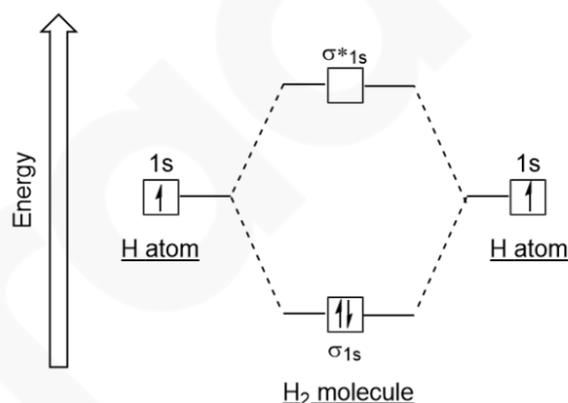
- Diatomic molecules are always in a linear fashion.
- For rotation and vibration, diatomic molecules have quantized energy levels.
- Many homonuclear diatomic molecules are rooted to the halogen series.

Homonuclear Diatomic Molecules

Diatomic Homonuclear Molecules are molecules that have only two atoms and are made up of a single nucleus. Due to the electronegativity difference of zero, the bond in a homonuclear diatomic molecule is non-polar.

Hydrogen molecule (H_2)

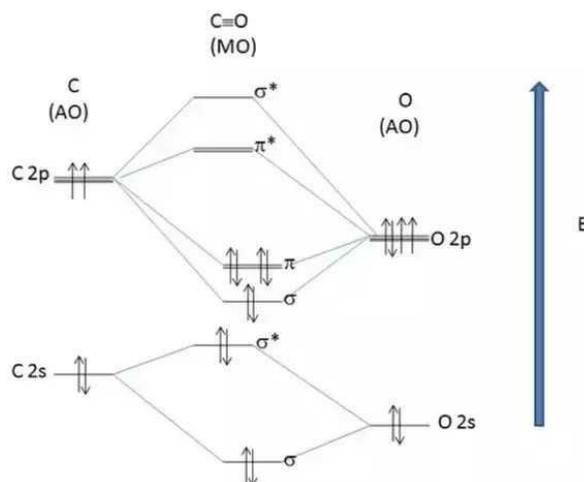
The formation of H_2 is the outcome of the union of two hydrogen atoms. Because each hydrogen atom has one electron in the 1s orbital, each hydrogen molecule has two electrons. Both of these electrons must be trapped in the lowest-energy molecular orbital. Pauli's Exclusion Principle dictates that these two electrons have opposite spins. The H_2 molecule's molecular orbital energy level diagram is :



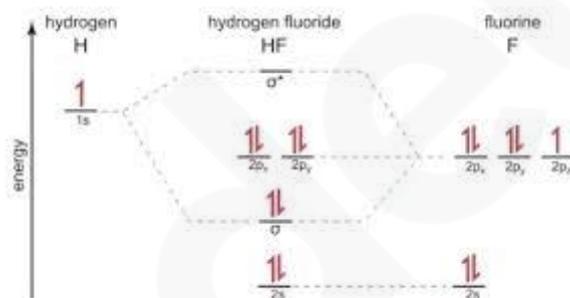
Heteronuclear diatomic molecules

Heteronuclear diatomic molecules are diatomic molecules containing two non-identical atoms. When atoms are not identical, the molecule is formed by merging unequally energetic atomic orbitals. As a result, each molecular orbital receives an uneven contribution from atomic orbitals, resulting in a polar bond.

Atomic orbitals of heteronuclear diatomic compounds only mix when their electronegativity levels are identical. Because the oxygen 2s orbital in carbon monoxide (CO) has a lower energy than the carbon 2s orbital, mixing is minimal. Because the molecule lacks a centre of symmetry, the g and u subscripts are no longer applicable.



Because the energy of 1s of hydrogen is comparable to 2p of fluorine, the hydrogen 1s orbital can interact with the fluorine 2p_z orbital to create a sigma bond in hydrogen fluoride (HF). The other electrons in the HF electron configuration remain in three lone pairs, and the bond order is one.



Difference between homo and hetero-nuclear diatomic molecules.

MOs for homonuclear diatomic molecules have equal contributions from each interacting atomic orbital, whereas MOs for heteronuclear diatomic molecules have varied contributions from each interacting atomic orbital.

If there is enough overlap between atomic orbitals, as dictated by their symmetries, orbital interactions that form bonding or antibonding orbitals in heteronuclear diatomics occur.

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