

27/5

Page-1

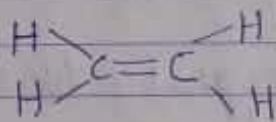
Molecular orbital diagram

BSc (H)

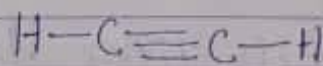
IIIrd part

A molecular orbital diagram or MO diagram, is a qualitative descriptive tool explaining chemical bonding in molecules in terms of Molecular orbital theory in general and the linear combination of atomic orbitals (LCAO) method in particular. A fundamental principle of these theories is that as atoms bond to form

2 unsaturated Hydrocarbon \rightarrow A hydrocarbon in which the two carbon atoms are connected by a double bond or a triple bond is called an unsaturated hydrocarbon. Ethene ($\text{H}_2\text{C}=\text{CH}_2$) and ethyne ($\text{HC}\equiv\text{CH}$) are two important unsaturated hydrocarbons, because ethene contains a double bond and ethyne contains a triple bond between two carbon atoms.



Ethene



Ethyne

A double bond is formed by the sharing of two pairs of electrons between the two carbon atoms whereas a triple bond is formed by the sharing of three electron pairs between two carbon atoms. The unsaturated hydrocarbon

27/5
Page-2

BSc (H) IInd part

more complex when discussing even comparatively simple polyatomic molecules, such as methane. MO diagrams can explain why some molecules exist and others do not. They can also predict bond strength, as well as the electronic transitions that can take place.

Qualitative MO theory was introduced in 1928, by Robert S. Mulliken and Friedrich Hund. A mathematical description was provided by contributions from Douglas Hartree in