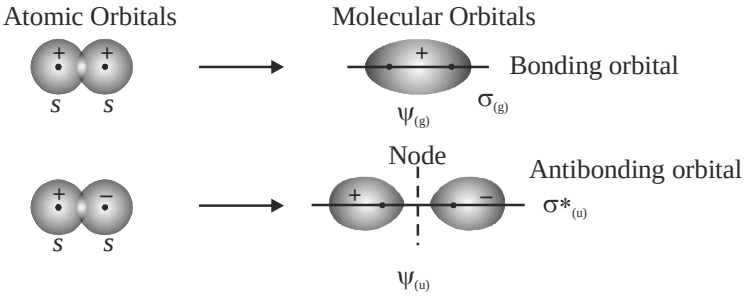
TYPES OF SYMMETRIES OF MO's

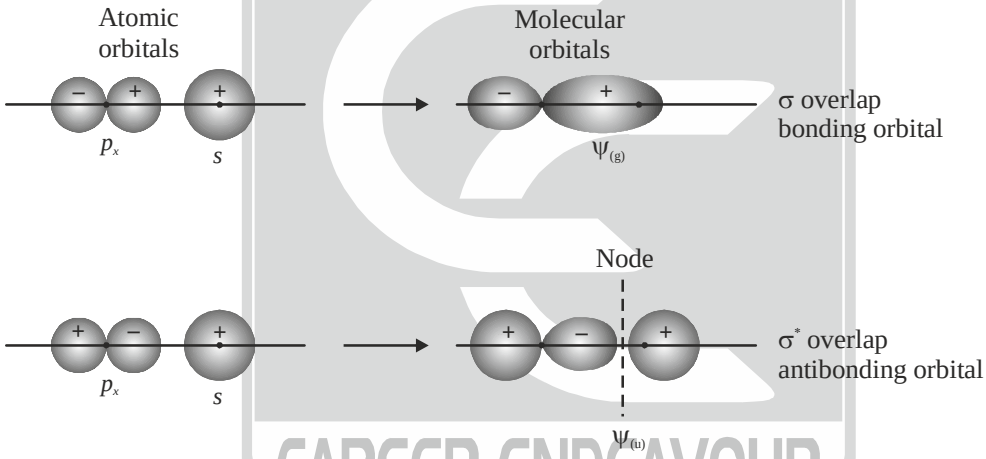
s-s combinations of orbitals:



s-s combinations of atomic orbitals

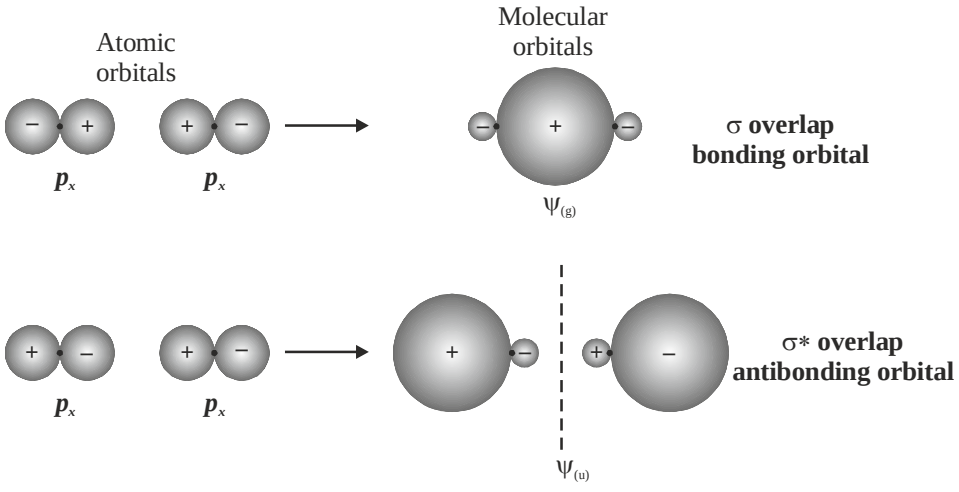
In the bonding MO there is increased electron density between the nuclei where as in the anti-bonding MO the electron density between the nuclui is zero (since the two lobes of opposite sign cancel the function). Both in the atomic orbital pair before interaction and tthe MO's formed after interaction, there is cylindrical symmetry around the bond axis i.e, any point on the orbital surface describes a circle as the MO is rotated around the bond axis. This circle is a plane perpendicular to the bond axis. All the points on such a circle have either a positive sign or negative orbital sign. There is no change of sign i.e, no node as we move over the circle. This is term cyclindrical symmetry and orbitals with cyclindrical symmetry are designated, σ, if they are bonding and σ^*, if they are antibonding.

s-p combinatinos of orbitals:

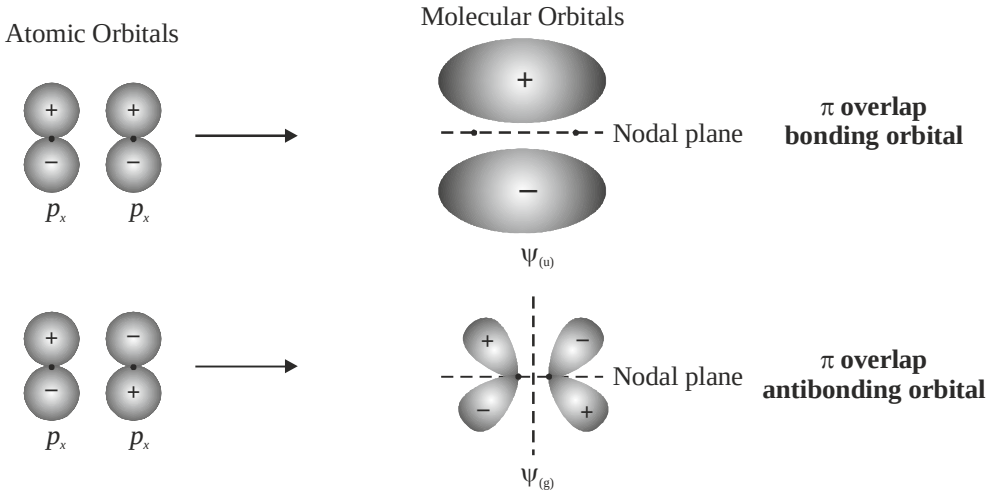


s-p combinatino of atomic orbitals

p-p combinations of orbitals:

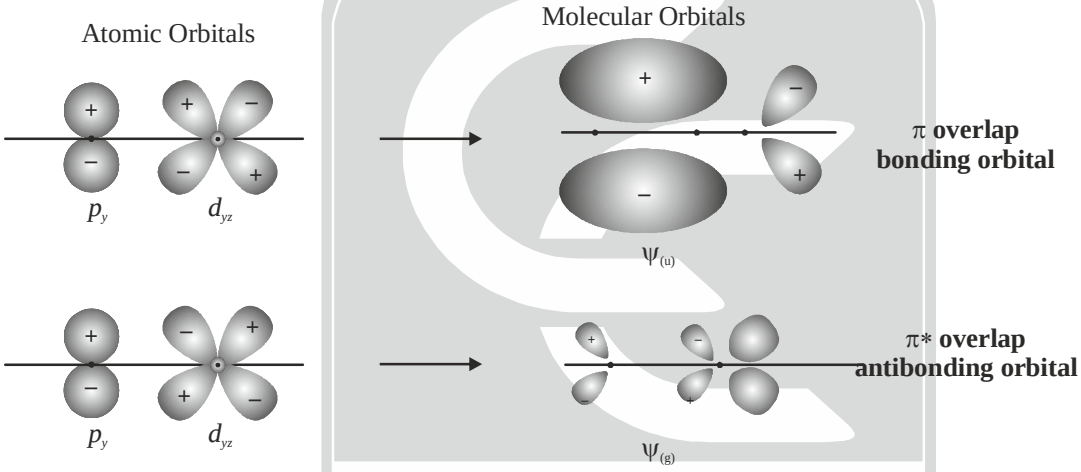


p-p combinations of atomic orbitals



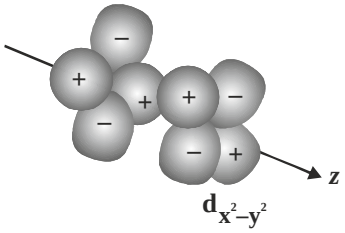
p-p combinations giving π bonding

p-d combinations of orbitals:



p-d combinations of atomic orbitals

d-d combinations of orbitals:



δ bonding by d-orbitals
(sideways overlap of two $d_{x^2-y^2}$ orbitals)

Non-bonding combinations of orbitals: In the combinations shown in the figure below any stabilization which occurs from overlapping + with + is destabilized by an equal amount of overlap of + with –. There is no overall change in energy, and this situation is termed non-bonding. It should be noted that in all these non-bonding cases the symmetry of the two atomic orbitals is different, i.e. rotation about the axis changes the sign of one.