

M.O. Theory

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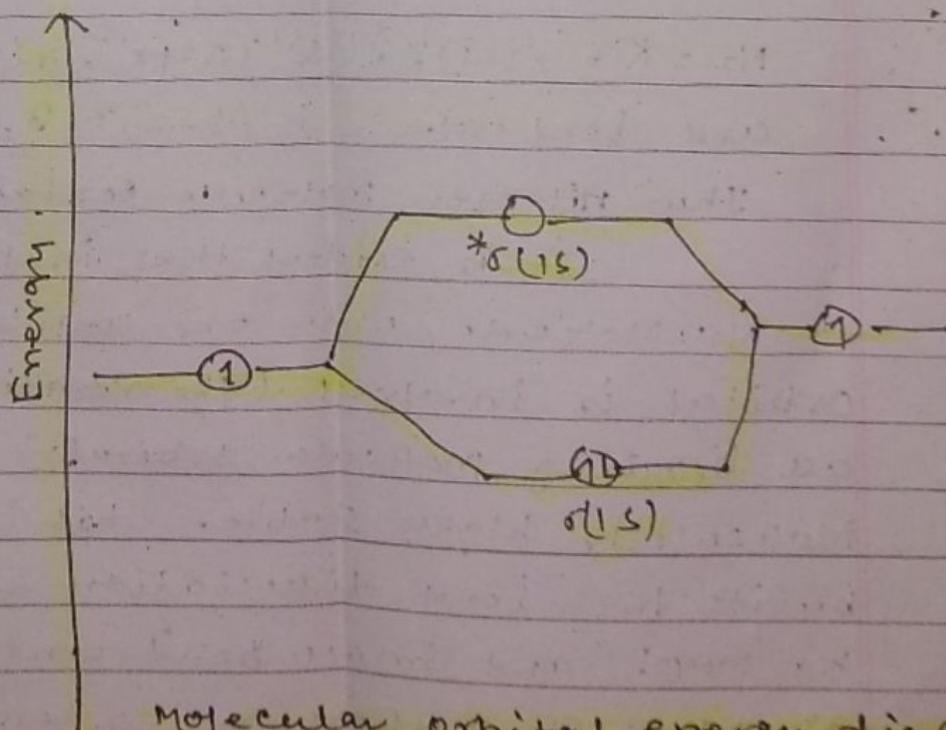
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Lecture Notes Series - 24

M.O. diagram of simple homonuclear

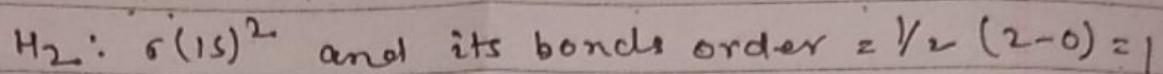
(H₂, N₂, O₂, F₂) Molecule

1. Hydrogen Molecule [H₂] : - It is formed by the combination of two hydrogen atoms. Each hydrogen atom has one electron in 1s orbital and therefore there are two electrons to be accommodated in Mo. Both these electrons would be accommodated in the r(1s) BMO. In accordance with Pauli's exclusion principle, these two electrons should have opposite spins. The molecular energy level diagram for H₂ molecule is presented in fig.



Molecular orbital energy diagram
of H₂ Molecule.

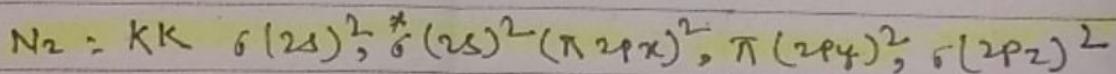
The electronic configuration of H₂ Molecule is thus,



This means that two hydrogen atoms are bonded together by a single bond. The bond dissociation energy of H₂ Molecule has been found to be 458 KJ Mol⁻¹ and bond length equal to 0.74 Å.

Nitrogen Molecule (N₂)

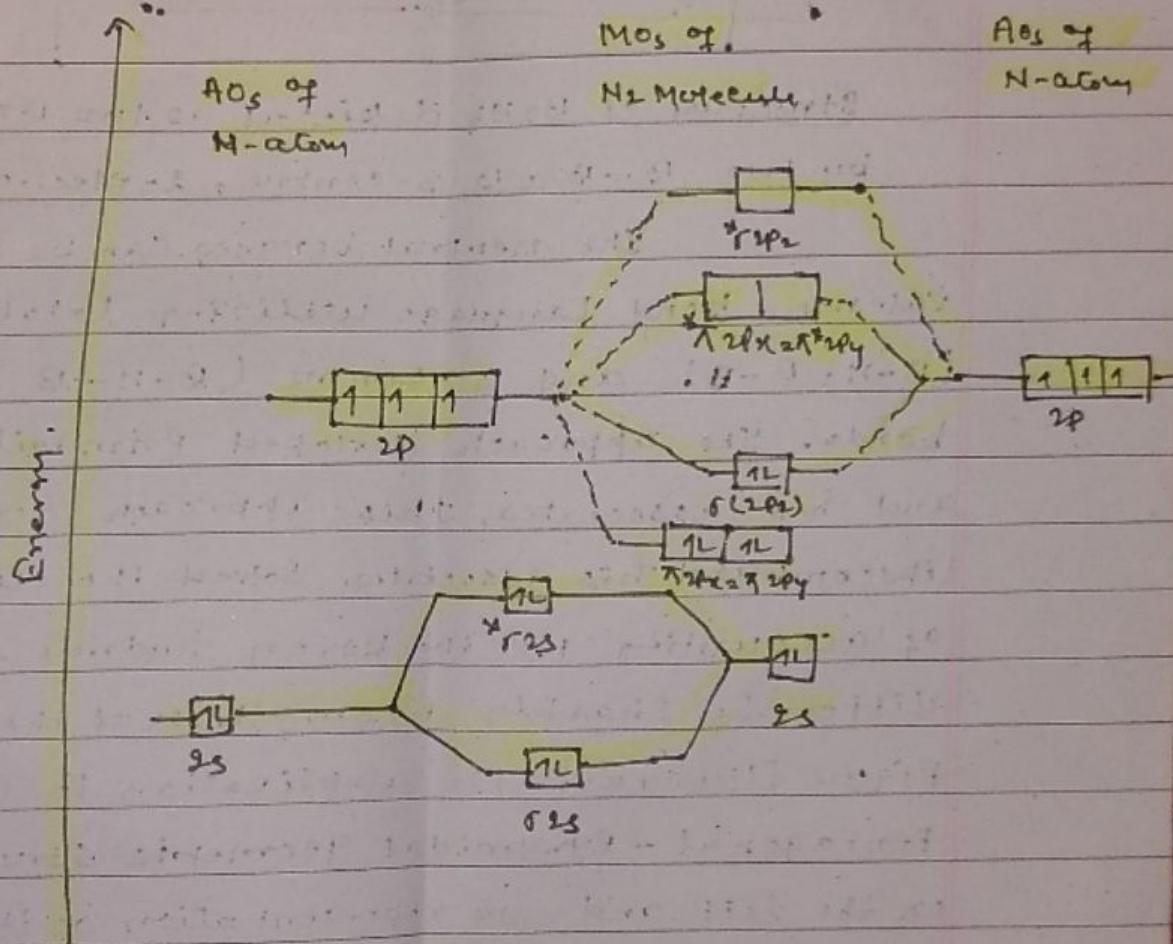
Consider, Next the formation of N₂ Molecule, The electronic configuration of Nitrogen (Z=7) is 1s², 2s², 2p³. The outer shell in this case contains 5 electrons. Thus there are 10 electrons to be accommodated in the Molecular orbitals of N₂. The electronic configuration of Nitrogen Molecule is thus



and bond order = $\frac{1}{2}(8-2) = 3$.

Thus Nitrogen Molecule contains a triple bond. It is evident that in the formation of N₂ Molecule, only one anti bonding molecular orbital is involved (the remaining four being all bonding Molecular Orbitals) Hence, the nitrogen Molecule is highly stable. This is confirmed by its high bond dissociation energy viz. 945 KJ Mol⁻¹ and small bond length equal to 1.10 Å. Also since there are no unpaired electrons

any orbitals. N_2 Molecule is diamagnetic.



M.O. diagram of N_2 Molecule

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