

Molecular Orbital Theory

(1)

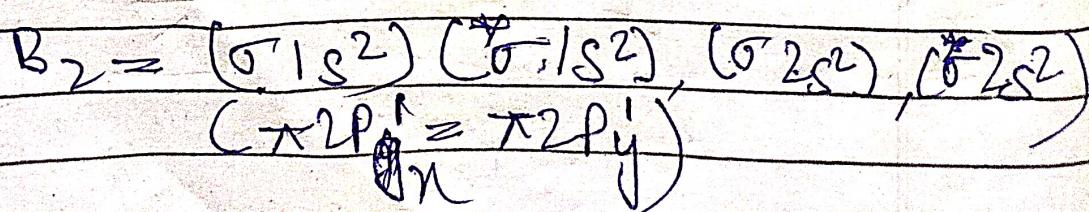
- Fails to Explain the formation of Coordination Compound
- Colour of Co-ordinate Compound
- Magnetic Behaviour, i.e Paramagnetic & Diamagnetic
- Bond Length, Bond Strength, Kinetic Stability & Thermal Stability

(2)

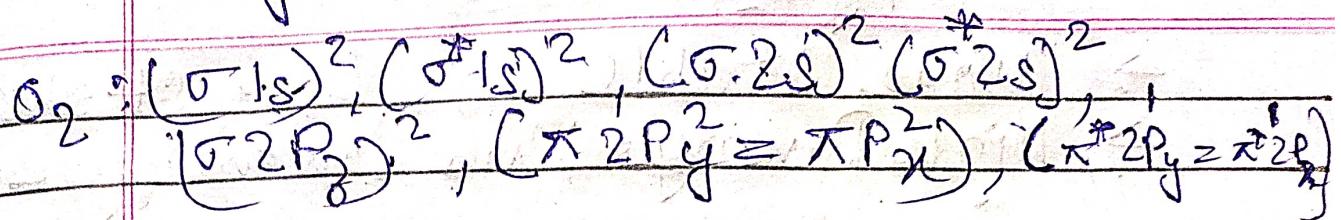
Molecular orbital is a polyatomic system, defined by its size, each having capacity of two electrons of opposite spin.

(3)

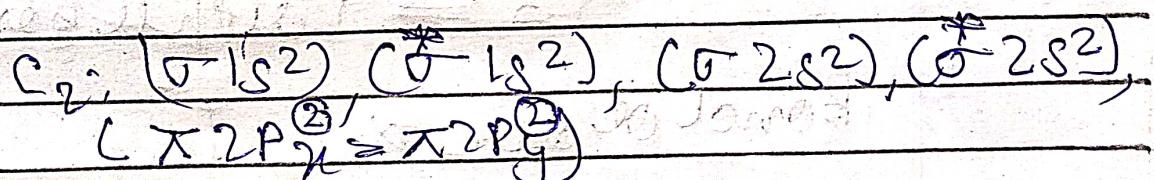
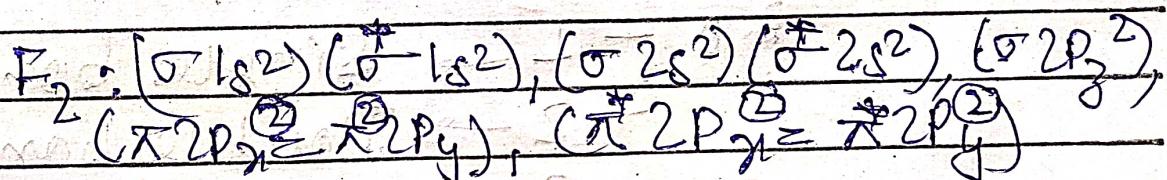
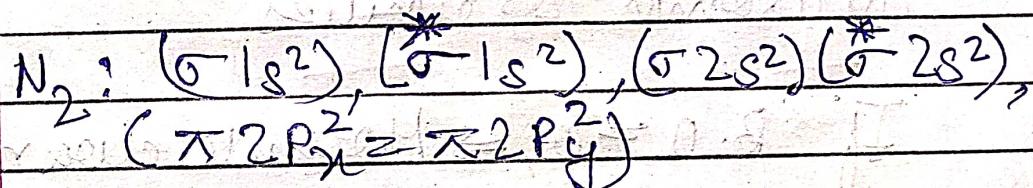
O_2 & B_2 are paramagnetic elements molecule in 2nd period. They are paramagnetic in Nature because of presence of two unpaired elements in bonding Molecular orbitals. So NOT



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④ N_2, F_2 and C_2 are diamagnetic in 2nd period, they are diamagnetic in nature because all of these atoms electrons are paired.



$Be_2 \rightarrow$ does not exist, as $B \cdot O = 0$

⑤ Difference b/w Bonding & Anti-bonding orbitals

② Bonding Orbital

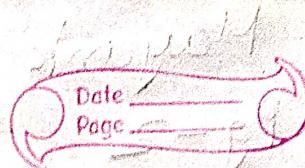
- lower in energy
- formed by additive overlapping
- $\Psi = \Psi_A + \Psi_B$

Anti bonding orbital

- High in Energy
- Formed by subtractive overlapping
- $\Psi = \Psi_A - \Psi_B$

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- More stable Less stable
→ High Density orbitals Low Energy orbitals

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Bond Order is an hypothetical concept, which gives us information about the stability of diatomic molecules.

If $B.O = 0$, \Rightarrow Molecule does not exist

$B.O = 1 \rightarrow$ Single bond
 $= 2 \rightarrow$ Double bond
 $= 3 \rightarrow$ Triple bond

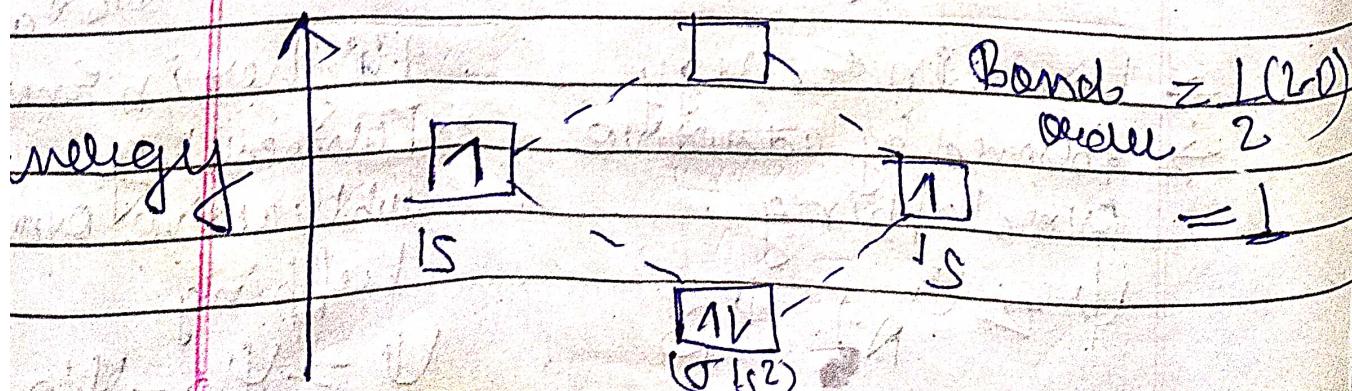
Bond Order \propto

Bond length

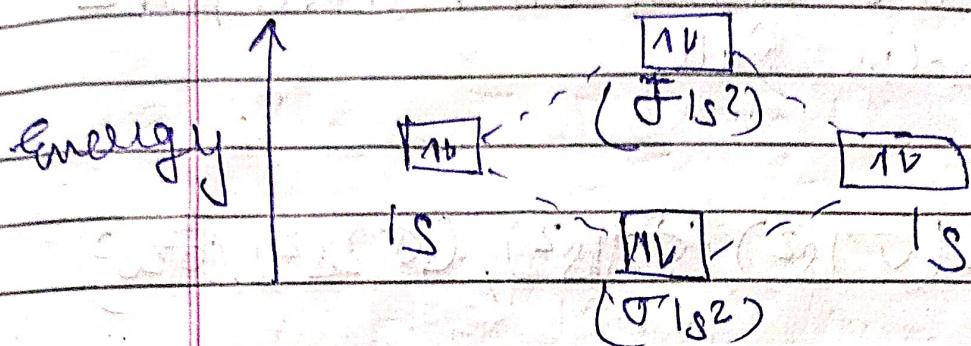
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Hydrogen form diatomic molecule, while helium forms monatomic

M.O diagram of H_2



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M.O. diagram of H_2 

$$\text{Bond Order} = \frac{1}{2} [2 - 2] = 0$$

∴ Does not Exist

LONG ANSWER

(b) Postulates of MOT

- (i) Atomic orbital of combining atoms overlap to form new orbitals called molecular orbitals.
- (ii) No. of atomic orbitals \geq No. of Molecular orbitals

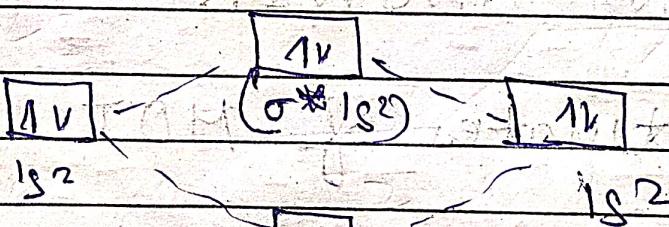
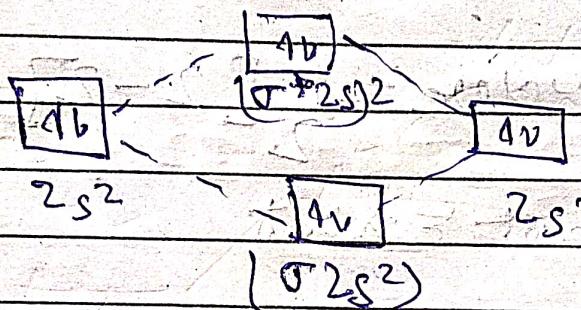
- Atomic orbital combined by Linear combination of atomic orbitals (LCAO)
- The atomic orbital must be of similar energy
- The atomic orbital must have similar shape & geometry.

→ It follows Aufbau principle,
Pauli's Exclusion Principle &
Kondo's Rule

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$$\text{Be} = (\sigma 1s^2), (\sigma^* 1s^2), (\sigma 2s^2), (\sigma^* 2s^2)$$

Energy ↑

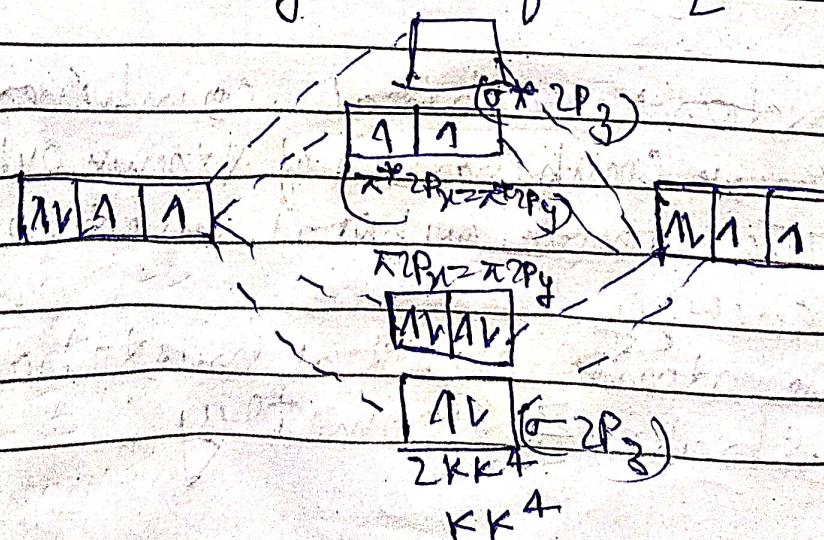


$$\text{Bond Order} = \frac{1}{2}(2-2) = 0$$

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M.O. diagram for O₂

Line



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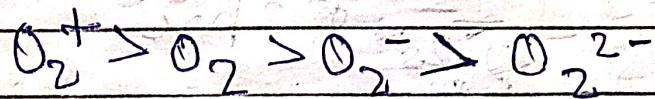
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$$\text{Bond order of } O_2 = \frac{1}{2} [10-6] = 2$$

$$\text{Bond order of } O_2^+ = \frac{1}{2} [10-5] = 2.5$$

$$\text{Bond order of } O_2^- = \frac{1}{2} [10-8] = 1.5$$

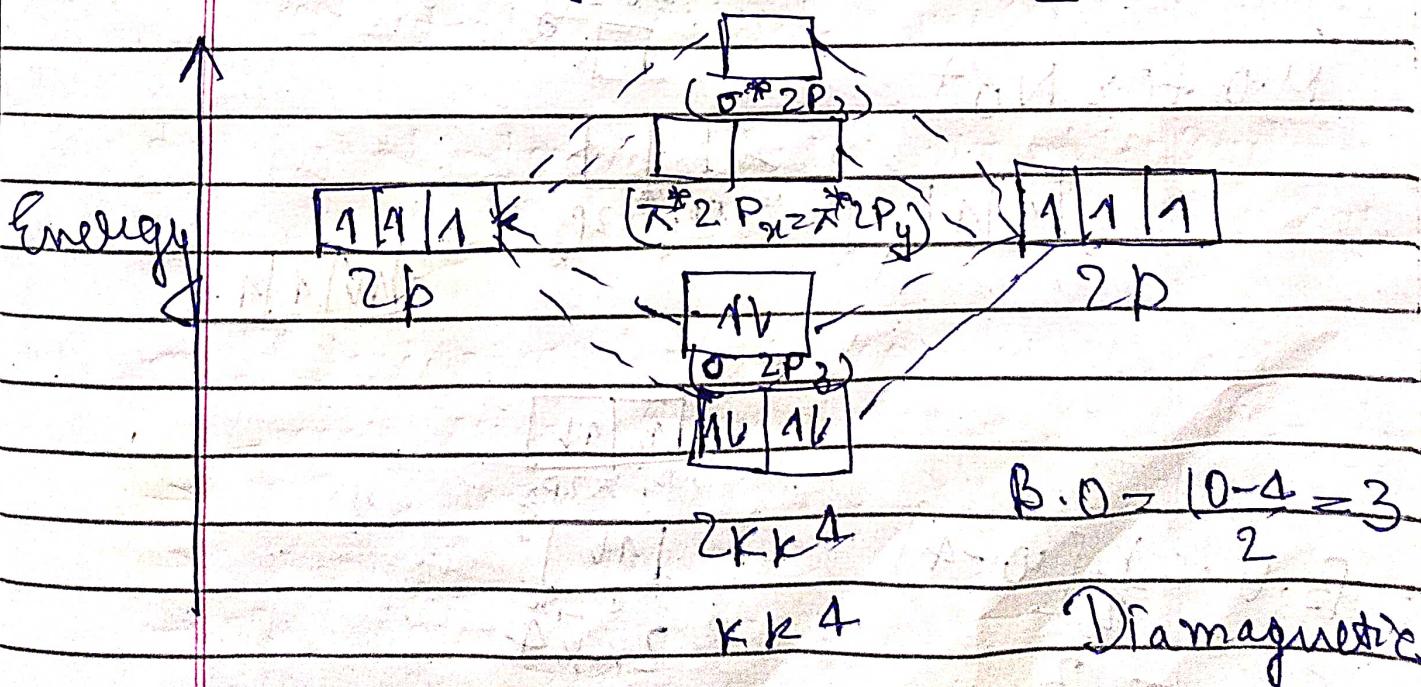
$$\text{Bond order of } O_2^{2-} = \frac{1}{2} [10-8] = 1$$



Since, O_2 , O_2^+ & O_2^{2-} are having unpaired e^- , so they are paramagnetic,

Whereas O_2^- does not have unpaired e^- , so Diamagnetic.

(4) M.O. diagram for N_2



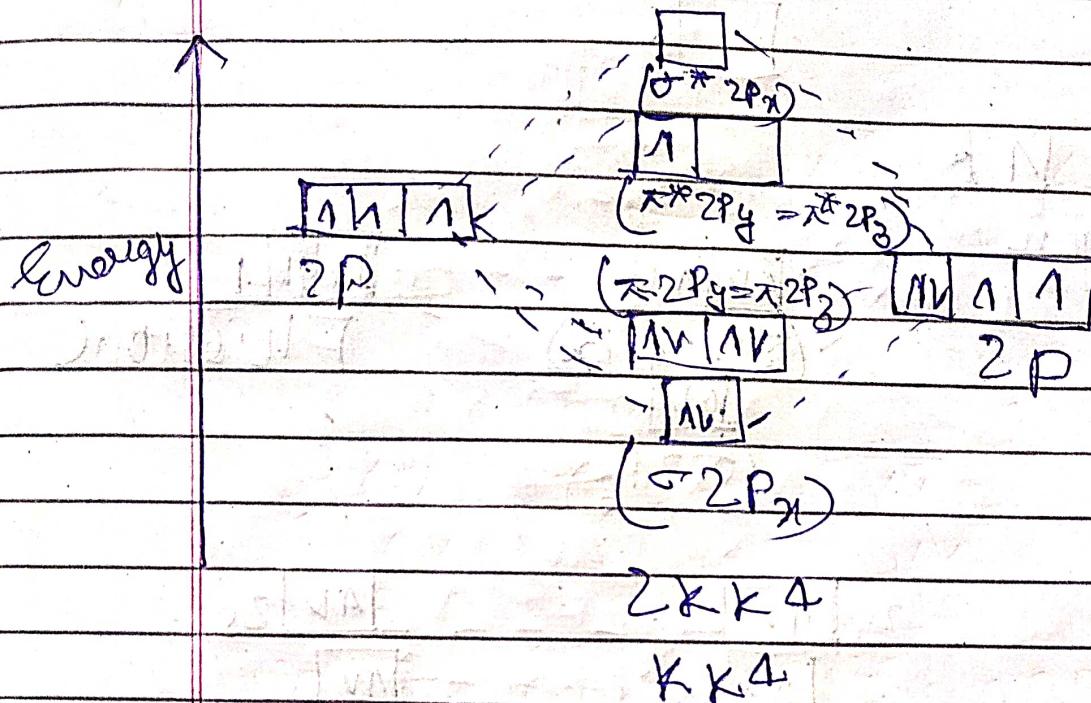
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⑤

M.O. diagram of a diatomic molecule NO



$$\text{Bond Order} = \frac{1}{2} [10 - 5] = 2.5$$

Paramagnetic

NO^+ molecule is more stable than NO molecule because formation of NO^+ from NO requires removal of one e^- from antibonding orbital.

$$\text{B.O} = \frac{1}{2} [10 - 4] = 3$$

B.O of $\text{NO}^+ >$ B.O of NO

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(8) MO for HF and HCl

Hydrogen



($\pi^2 p_{n_z} \pi^2 p_{z_c}$)

[AV]

($\sigma^2 p_3$)

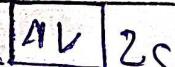
Fluorine

Energy



[1V]

LS



[1V]

LS

Electronic Configuration $n1s^2, n2s^2, \sigma^2 s^2, n2p^2_n, n2p^2_y$

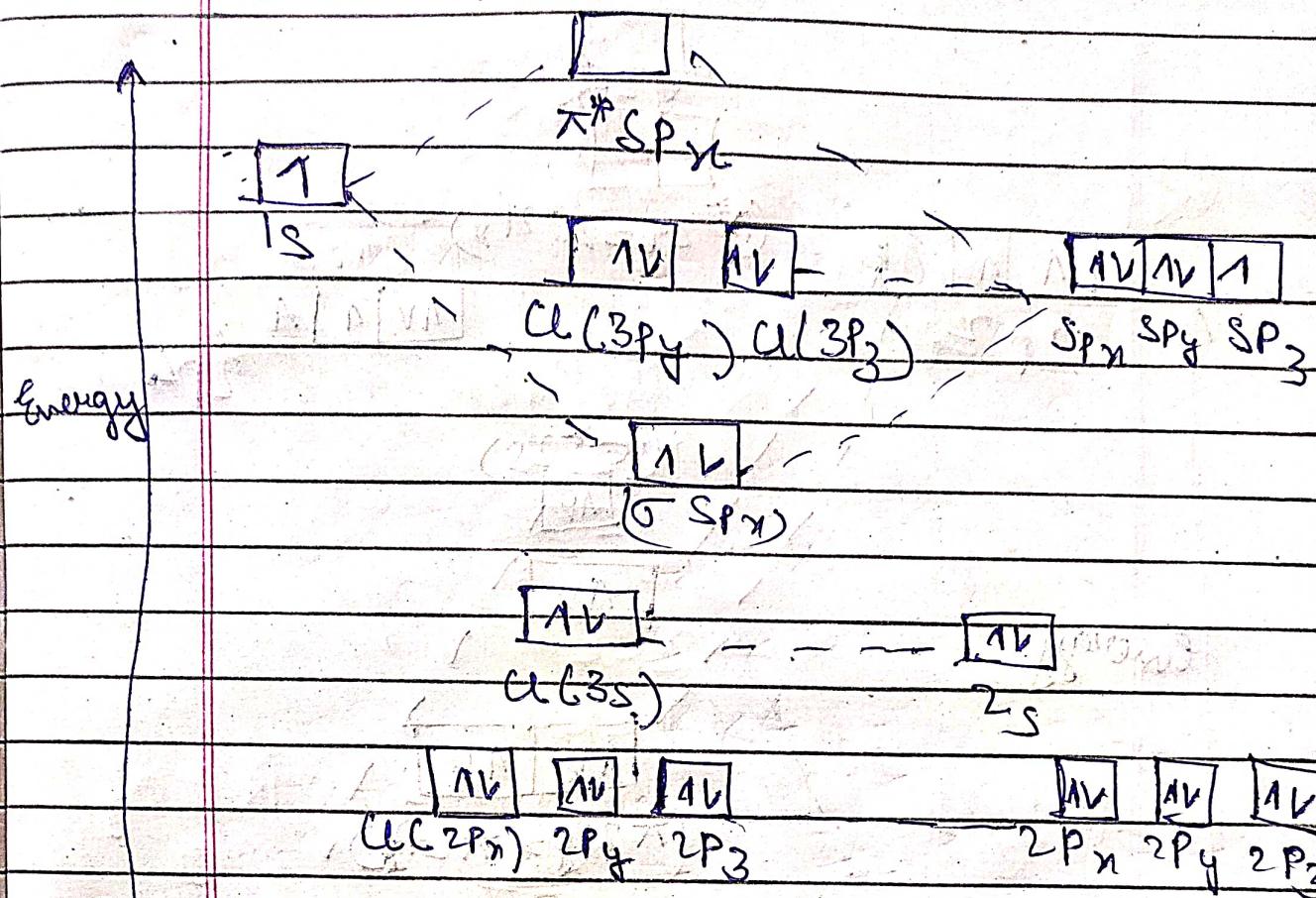
Bond Order $\Rightarrow [2 - 0] = 1 \Rightarrow$ Diamagnetic

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M.O diagram for HCl



genuine

H-atoms

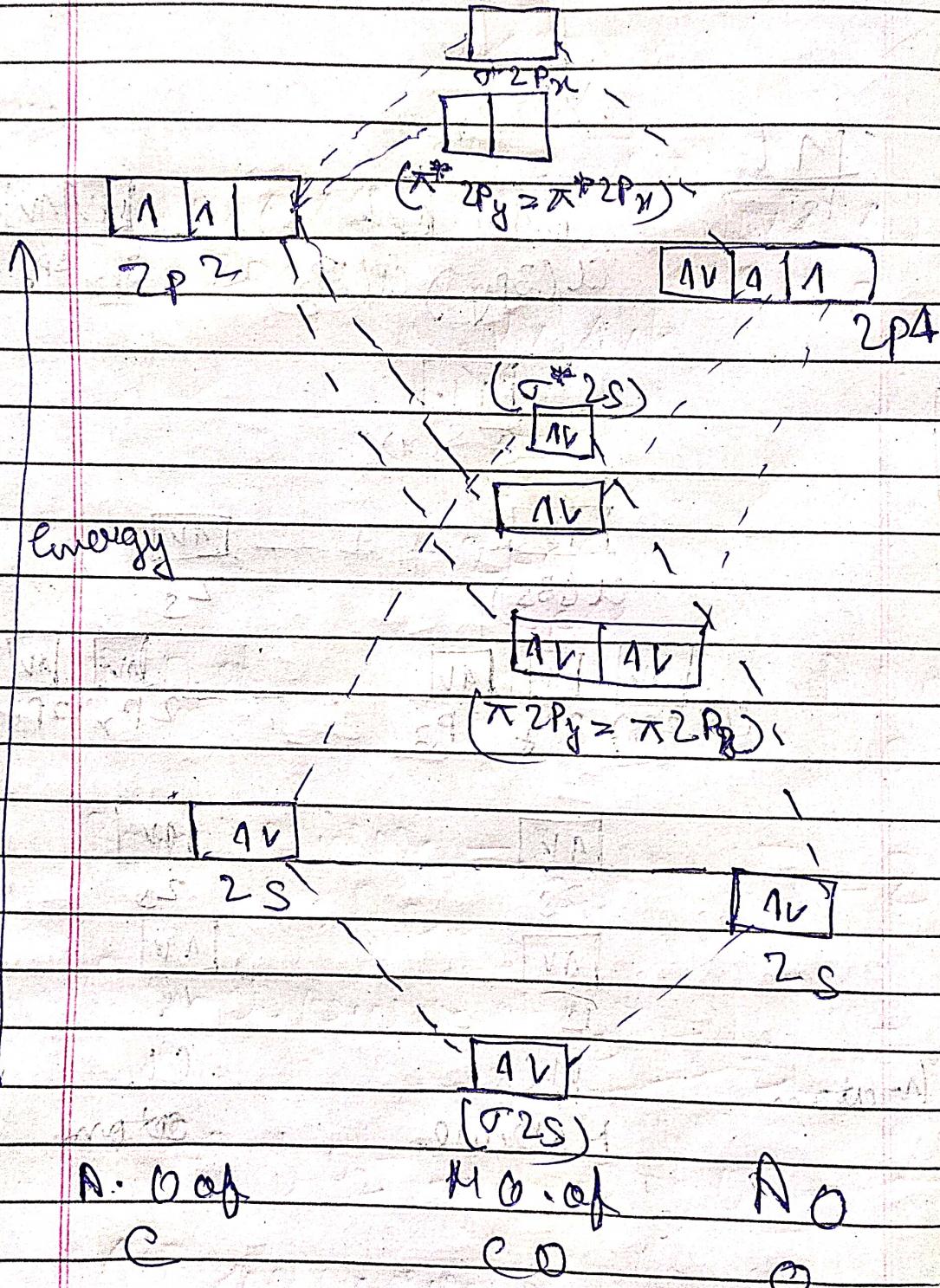
HCl
Molecule

Cl
Atom

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(7) H₂O Molecules of C₂O



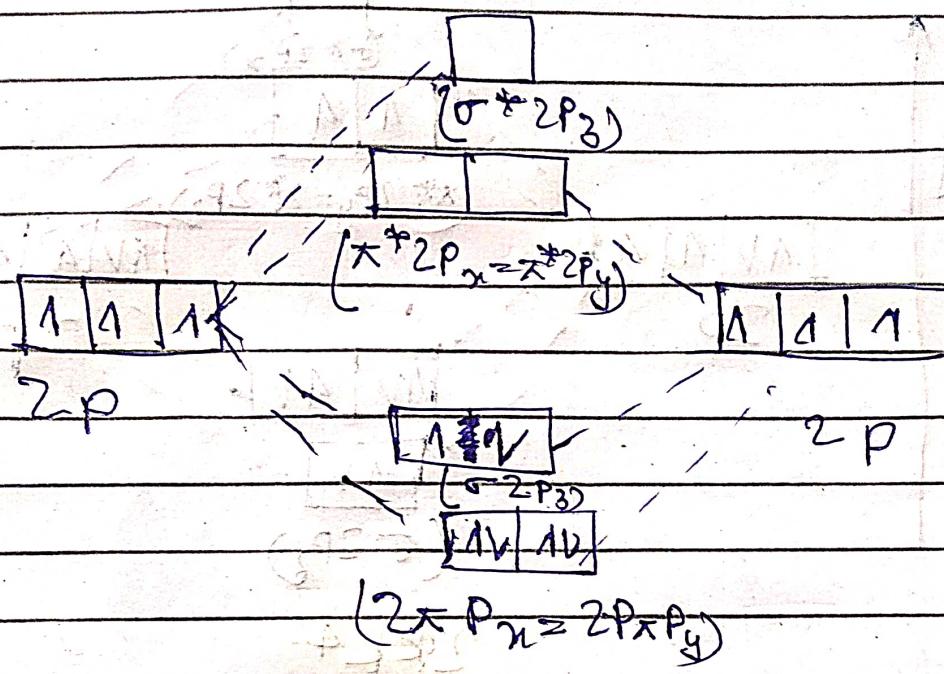
Bond Order = $\frac{1}{2} [10 - 4] = 3$

Diamagnetic

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(8) M.O diagram of N_2



M.O of N M.O of N_2 M.O of N

$$\text{Bond Order of } N_2 = \frac{1}{2} [10 - 4] = 3$$

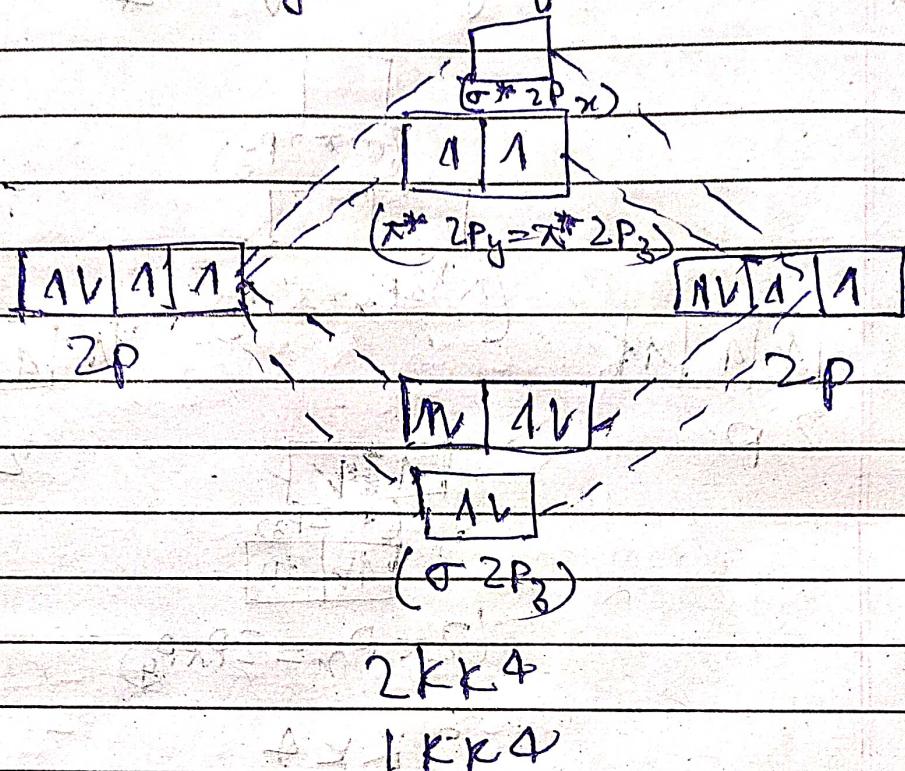
$$\text{Bond Order of } N_2^+ = \frac{1}{2} [9 - 4] = 2.5$$

Since, Bond Order & Bond Energy

N_2 has more bond energy or dissociation energy than N_2^+

M.O diagram of O_2

Energy



A.O of O M.O for O_2 A.O of O

$$\text{Bond Order} = \frac{1}{2} [10 - 6] = 2$$

$$\text{Bond Order of } O_2^+ = 1, [10 - 8] = 1$$

$$\therefore \text{BO of } O_2^+ > \text{BO of } O_2$$

\uparrow Bond Order \propto Bond Energy

Therefore, O_2^+ has more dissociation energy than O_2

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Band Theory

- Q) What is metallic bond? Explain it with the help of band theory.

Sol-① Metallic bonding is a type of chemical bonding that arises from the electrostatic and positively charged metal ions. It may be described as the sharing of free electrons among a structure of positive charged ion.

Metals conduct electricity with the help of valence electron present in them, the atomic orbitals of the metal having same energy combine to form molecular orbital which are close in energy to each other to form a band. Let consider a metal having an infinite number of atoms. They will form an infinite no. of molecular orbitals. To close together they blur into one another forming a band.

Let us take the example of Sodium.
 $\text{Na} \rightarrow 1s^2, 2s^2, 2p^6, 3s^1$: It has one unpaired electron in 3s level.

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The 3s atomic orbital of Sodium overlaps with another such orbital of same energy to form molecular orbital.

Molecular orbitals holds the atoms together and forms a new compound with the help of bond within same energy orbitals.

- ② How metallic bond is different from ionic and covalent bond? Explain it on the basis of MOT?

Ans ②

Metallic bond is different from Ionic or covalent bond because metals are electropositive in nature.

Ionic bond is formed b/w electropositive and electronegative elements. While metallic bond is formed b/w electropositive elements.

Metals can not combine with covalent bond because it is held with weak van der waals force while metallic bonds are strong.

③ When molecular orbital theory extended to solids is also referred as band theory.

④ No. of atoms in the cluster increases the spacing b/w the energy level of valence orbitals decreases.

⑤ In successive combination of atomic orbital for e.g. Na_2 atom, if two atomic orbitals overlap one bonding & anti-bonding MO's are formed, and both $\rightarrow \text{BO}$, Since

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Only half the MO's 3s valence bonds are filled in B MO's. It requires very small amount of energy to excite one e⁻ to an conduction MO, so c⁻ have high mobility & that is why metal have high thermal electrical conductivity.

The band of energy levels occupied by valence e⁻ is called valence band.

The next higher band above the valence band is conduction band.