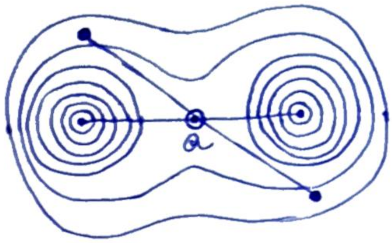
NAME: Priyanshu Mahato

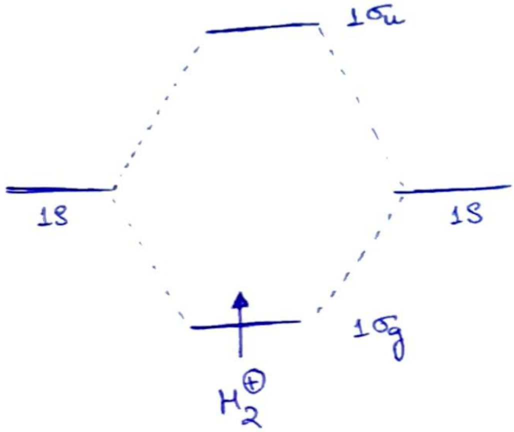
Roll No.: pm21ms002

CH1101

Assignment-5

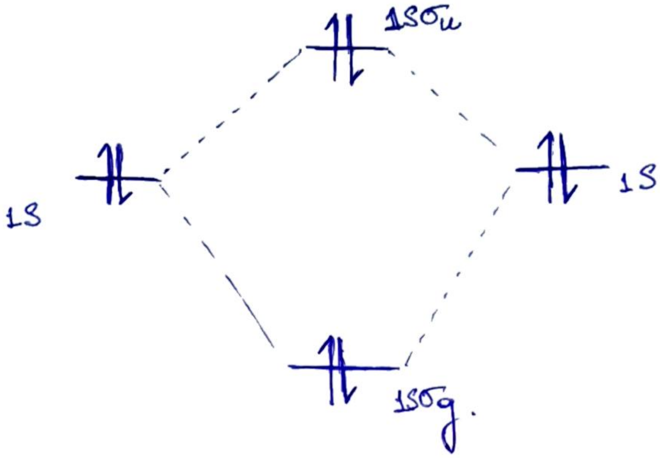
Q1. $H_2^{\oplus}$ MO Diagram:





Symmetry Labels: σ_g and σ_u, where g represents gerade and u represents ungerade. If 'a' is a pt. on the middle of the internuclear axis, then MO is symmetric/gerade if the sign remains same on both sides and asymmetric/ungerade if the signs become opposite on both sides.

Q2.

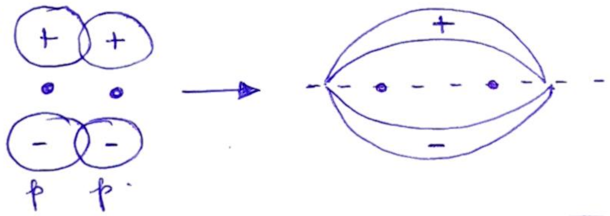


In this MO, the no. of ABMO is equal to BMO, due to which Bond Order (BO) = 0, so the He_2 molecule tends to become unstable and prefers to stay as 2He. This is why He_2 is an unobserved species.

For He_2^{2+}, electrons will only be filled in the BMO's. Thus, it'll be more stable (and the overlap integral $S > 0$) and will exist.

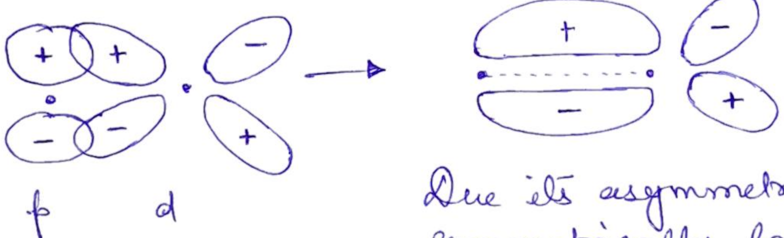
For H_2^{2-}, there'll be same no. of electrons in Bonding & Anti-Bonding MO's, so, the molecule would be unstable and would ~~rather~~ not be observed naturally.

Q3. (a)



π_g.

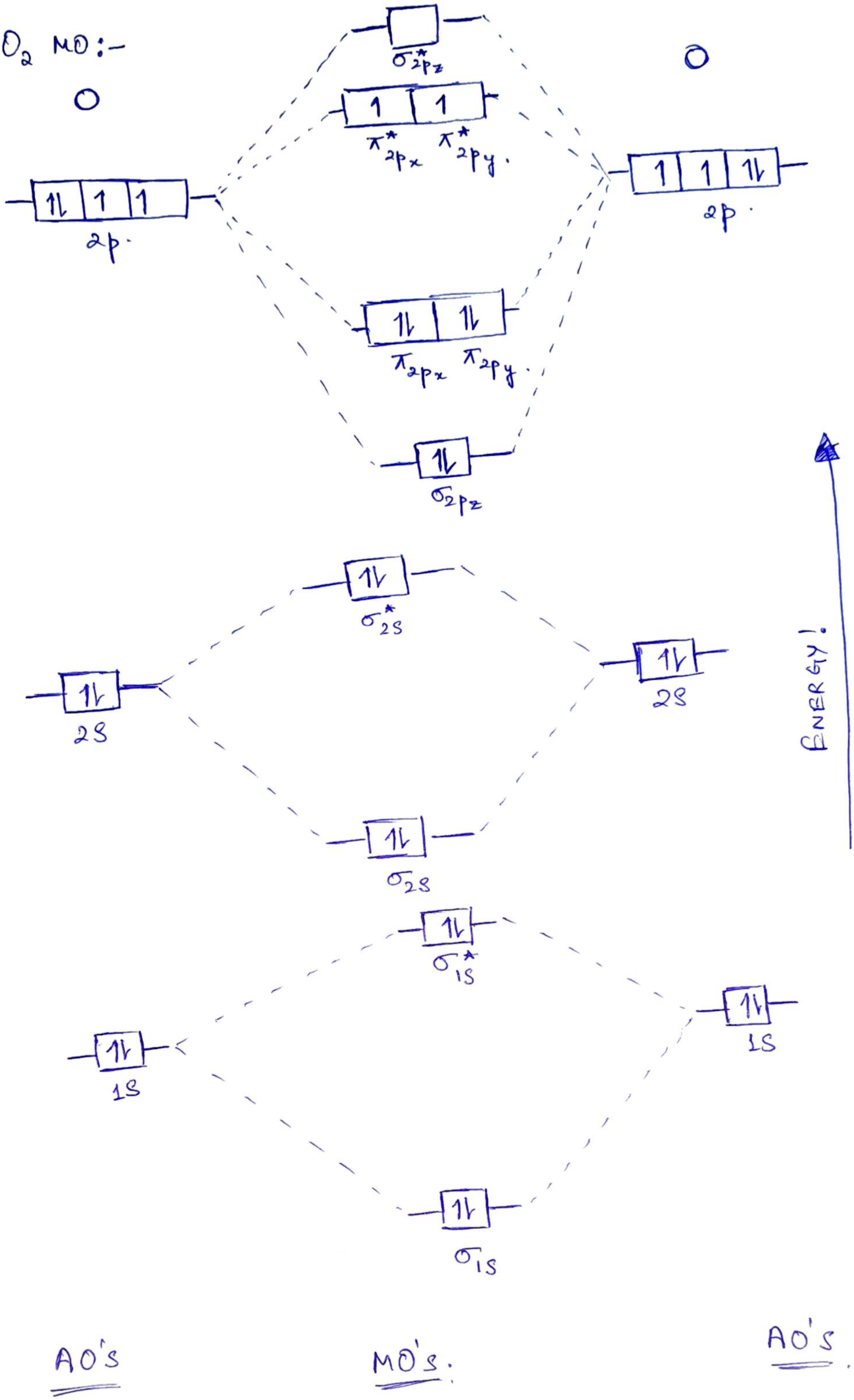
(b)



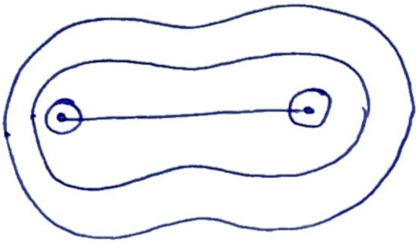
~~π_g~~ π

Due its asymmetry, it can't be symmetrically labelled.

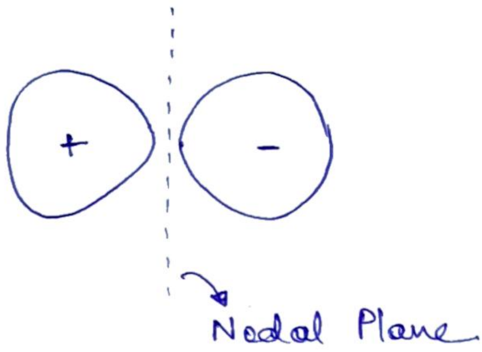
Q4. O_2 MO:-


O
O
$\sigma^*_{2p_z}$
$\pi^*_{2p_x}$ $\pi^*_{2p_y}$.
2p.
2p.
π_{2p_x} π_{2p_y}.
σ_{2p_z}
σ^*_{2s}
2s
2s
ENERGY!
σ_{2s}
σ^*_{1s}
1s
1s
σ_{1s}
AO's
MO's.
AO's.

$\sigma_g \rightarrow$

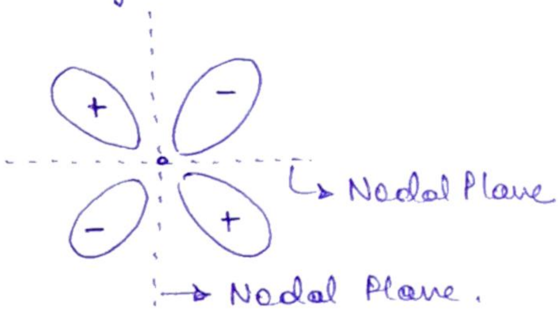


$\sigma_u \longrightarrow$

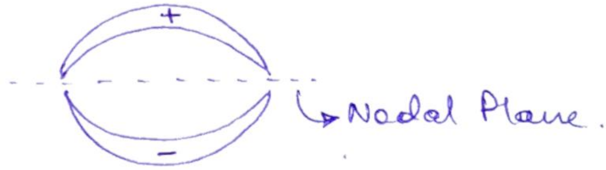


Although σ_g and σ_u are occupied, they make little to no contribution in O_2 bonding as ~~[illegible]~~ Orbital Contraction is very large due to which the overlap integral (S) tends to zero i.e., they do not intersect significantly.

π_g^* O_2



π_u O_2 .



O_2 exists in 3 states viz. 1 Triplet and 2 excited states. In this, the change occurs only in the π_u^* orbital.

(i) Triplet (Ground State) : π_u^* : $\underline{1}$ $\underline{1}$

(ii) Singlet (1st excited state) : π_u^* : $\underline{1\downarrow}$ _

(iii) Singlet (2nd excited state) : π_u^* : $\underline{1}$ $\underline{\downarrow}$

The visible change is mostly in the spin of the electrons.

●

Q5. There are 3 spin-states of O_2.

	GROUND STATE	1st EXCITED STATE	2nd EXCITED STATE
HOMO :	$\underline{1}\,\underline{1}$	$\underline{1\downarrow}$ _	$\underline{1}\,\underline{\downarrow}$

→ We observe luminiscence during generation of

● singlet oxygen because it is in excited state & have a very high energy which makes it unstable so release the energy as photons which cause chemical luminescence.

Q6. $CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$

Literature value of ΔH of $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$ = 460 kJ/mol

Predicted value of ΔH for combustion of CH_4 = 460 × 2
= 920 kJ mol^{-1}