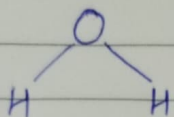
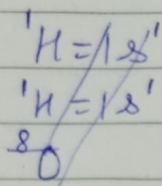


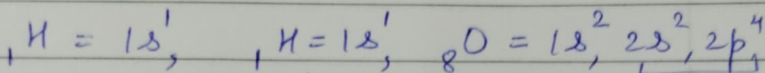
Molecular Orbital Diagram for H_2O (water)



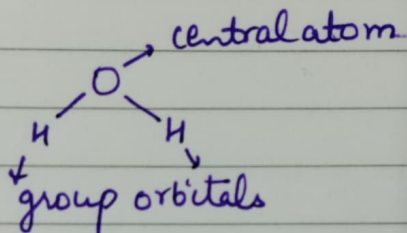
Bent shaped molecule
Point group: C_{2v}



Electronic configuration:

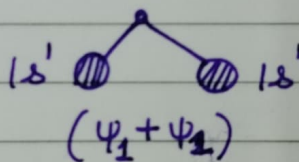


Only $2s$ & $2p$ will participate in bonding with $1s$ of two hydrogen atoms.



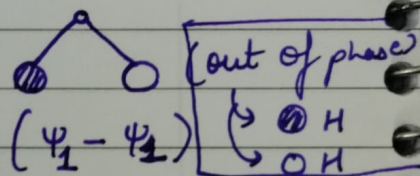
Possible Bonding:

Group orbitals \rightarrow



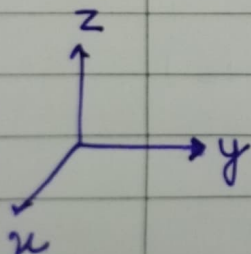
Addition
overlap

(Both hydrogens are in
same phase \odot)

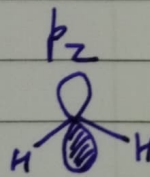
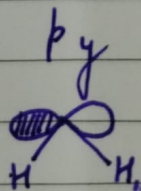
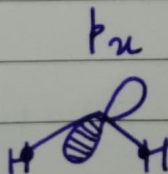


Subtraction
overlap

Orbitals of Oxygen: $\rightarrow 2s^2$



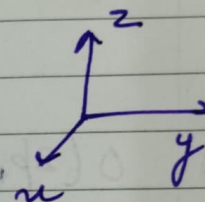
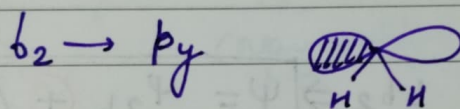
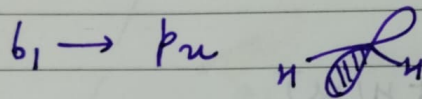
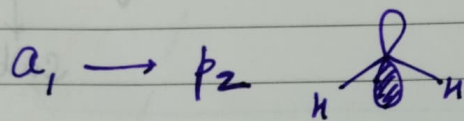
$2p \rightarrow$



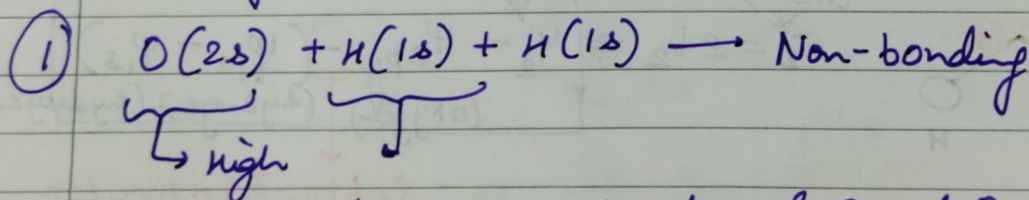
p-orbitals of Oxygen →

Character Table for H_2O (C_{2v}) point group

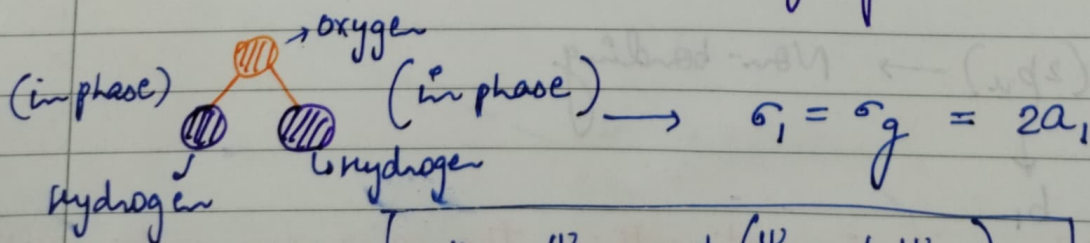
C_{2v}	E	C_2	σ_{xz}	σ_{yz}		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz



Possible Bonding between Hydrogen & Oxygen:

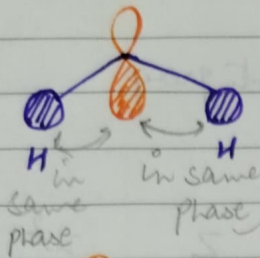


Energy difference so 1s of H & 2s of O either do not overlap or have the possibility of partial overlapping.



$$\boxed{\psi_1 = \psi_{2s}(\text{oxygen}) + (\psi_{1s} + \psi_{1s})(\text{hydrogen})} \rightarrow \text{Addition overlap}$$

(2) $O(2p_z) + H(1s) + H(1s)$

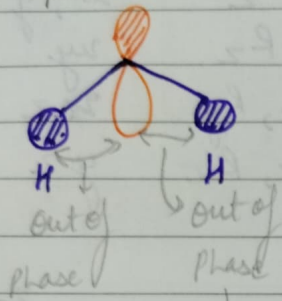


$$\sigma_3 = 3a_1 \Rightarrow$$

$$\psi_3 = \psi_{2p_z} + (\psi_{1s} + \psi_{1s})$$

(oxygen) (hydrogen) (hydrogen)

Addition overlap



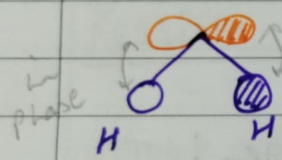
$$\sigma_3^* = 4a_1 \Rightarrow$$

$$\psi_3^* = \psi_{2p_z} - (\psi_{1s} + \psi_{1s})$$

(oxygen) (hydrogen) (hydrogen)

Subtraction overlap

(3) $O(2p_y) + H(1s) + H(1s)$



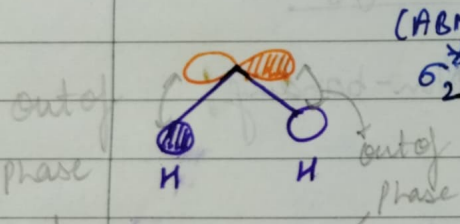
$$\sigma_2 = 1b_2 \Rightarrow$$

(BMO)

$$\psi_2 = \psi_{2p_y} + (\psi_{1s} - \psi_{1s})$$

(oxygen) (hydrogen) (hydrogen)

Addition overlap



$$\sigma_2^* = 2b_2 \Rightarrow$$

(ABMO)

$$\psi_2^* = \psi_{2p_y} - (\psi_{1s} - \psi_{1s})$$

(oxygen) (hydrogen) (hydrogen)

Subtraction overlap

(4) $O(2p_x) \rightarrow$ Non-bonding

$$b_1$$

(Since it is not getting the same symmetry orbital from hydrogen so it will go into non bonding state)

$$\psi_4 = 1b_1 \Rightarrow$$

