MO digram of CO_2

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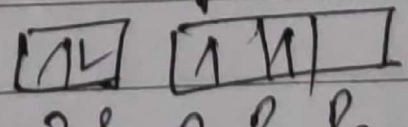
Carbon dioxide is a triatomic linear molecule in which carbon atom is a central atom and oxygen atom is peripheral atom.

$$O \overset{\pi}{=} C \overset{\pi}{=} O$$
$$\sigma \qquad \sigma$$

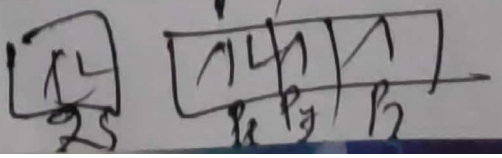
① Firstly orbital of oxygen atom combine together to form group orbital since in oxygen more P orbitals are combine together to form more group orbitals.

② Then group orbitals combine with matching symmetry of orbitals to form molecular orbitals.

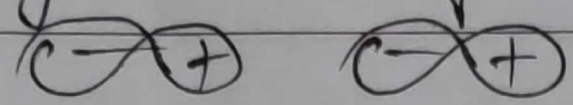
$C-(6) - 1s^2 2s^2 2p^2$



$O-(8) - 1s^2 2s^2 2p^4$

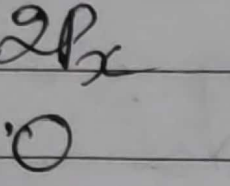


only 2p orbital of oxygen combine together to form group orbital



1)

$2p_x$ $2p_x$



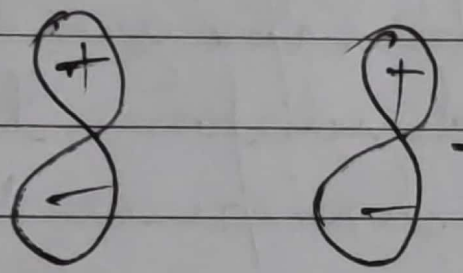
Substraction $\psi_2 = \psi_{2p_x} - \psi_{2p_x}$

O_1 O_2

addition $\psi_1 = \psi_{2p_x} + \psi_{2p_x}$

O_1 O_2

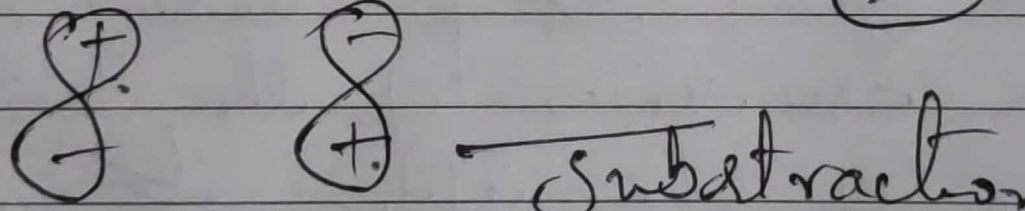
2)



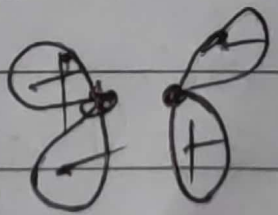
$2p_z$ $2p_z$

addition $\psi_3 = \psi_{2p_z} + \psi_{2p_z}$

O_1 O_2



Substraction



$\psi_4 = \psi_{2p_z} - \psi_{2p_z}$

O_1 O_2

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3) addition

$\psi_S = \psi_{2p_y} + \psi_{2p_y}$

$O_1 \quad O_2$

subtraction

$\psi_\sigma = \psi_{2p_y} - \psi_{2p_y}$

$O_1 \quad O_2$

$2s + \psi_1 \begin{cases} \sigma_S^* \\ \sigma_S \end{cases}$

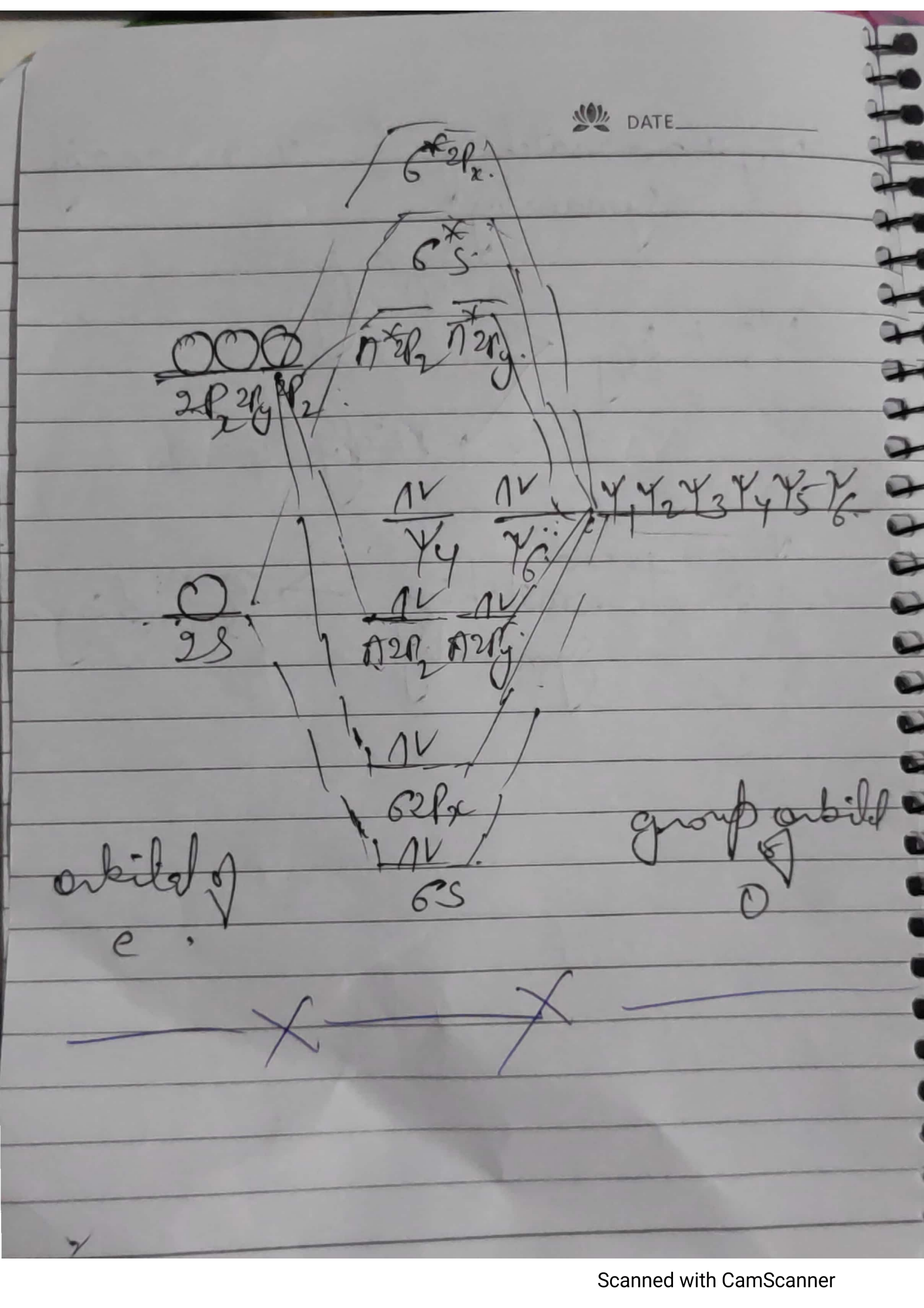
$2p_x + \psi_2 \begin{cases} \sigma^*_{2p_x} \\ \sigma_{2p_x} \end{cases}$

$2p_z + \psi_3 \begin{cases} \pi^*_{2p_z} \\ \pi_{2p_z} \end{cases}$

ψ_4 + no matching symmetry → non bonding

ψ_5 + $2p_y$ → $\pi^*_{2p_y}$ or π_{2p_y}

ψ_6 + no matching symmetry → non bonding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σ*2p_x
σ*s
π*2p_z π*2p_y
2p_z 2p_y 2p_z
ψ4 ψ5
ψ1 ψ2 ψ3 ψ4 ψ5 ψ6
2s
σ2p_z σ2p_y
σ2p_x
σs
orbital
e.
group orbital
O