

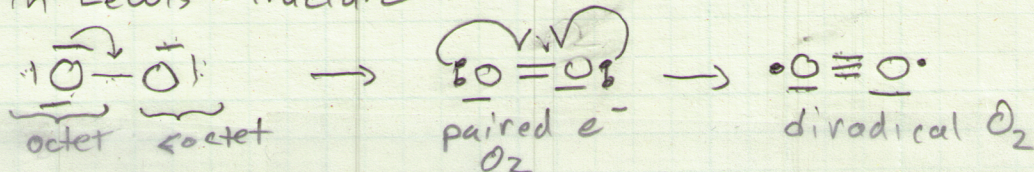
* DIRADICAL *

using diatomic oxygen (O_2) to demonstrate the relationship among fundamental concepts

- ① Lewis structure construction
- ② Atomic orbital e^- configuration using Aufbau and Pauli Exclusion Principles and Hund's Rule
- ③ How these Atomic orbitals are used to construct MOs (molecular orbitals)
- ④ How to fill MOs analogously using

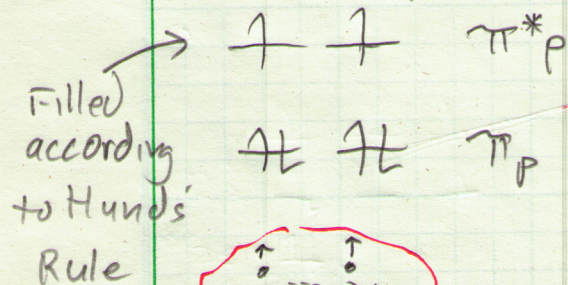
O_2
Lewis structure
neutral

- ① Each O atom has 6 valence e^- s
there are two O in O_2 $\therefore$ 12 valence e^- must be visible in Lewis structure

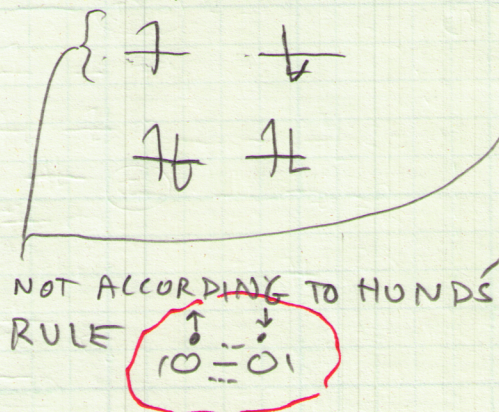


Let's Look at Relative Energies.

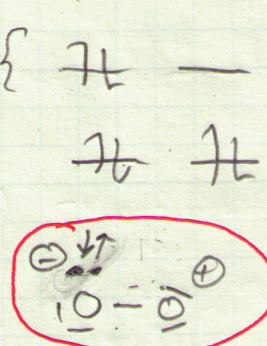
TRIPLET OXYGEN



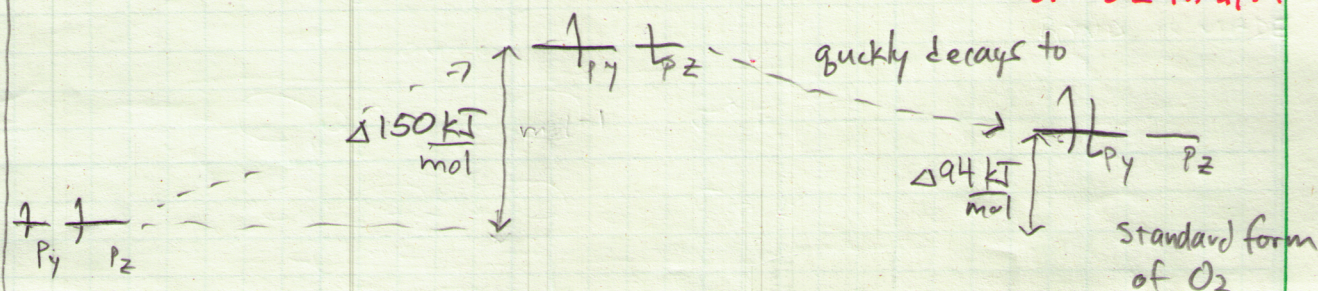
SINGLET OXYGEN



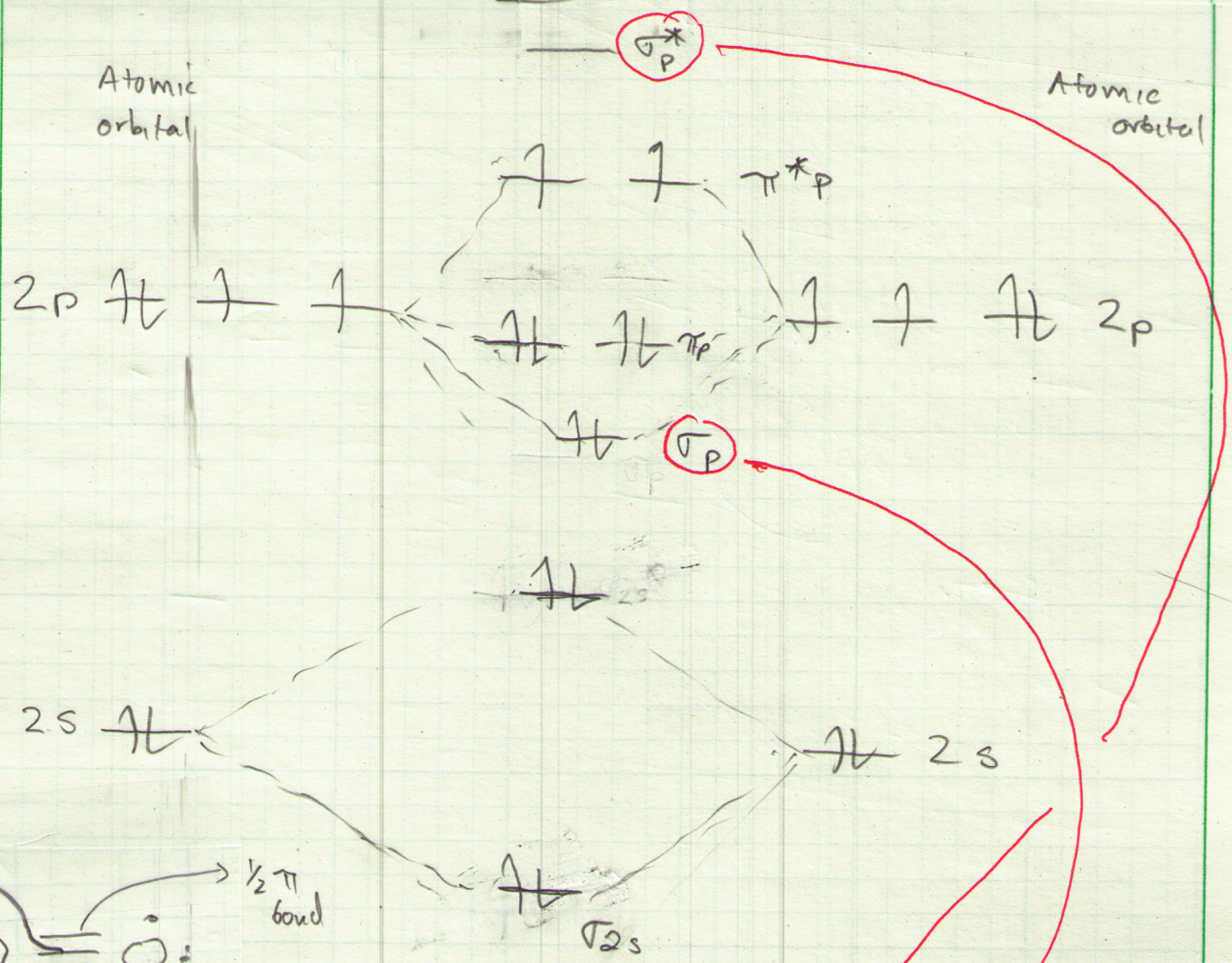
SINGLET O_2



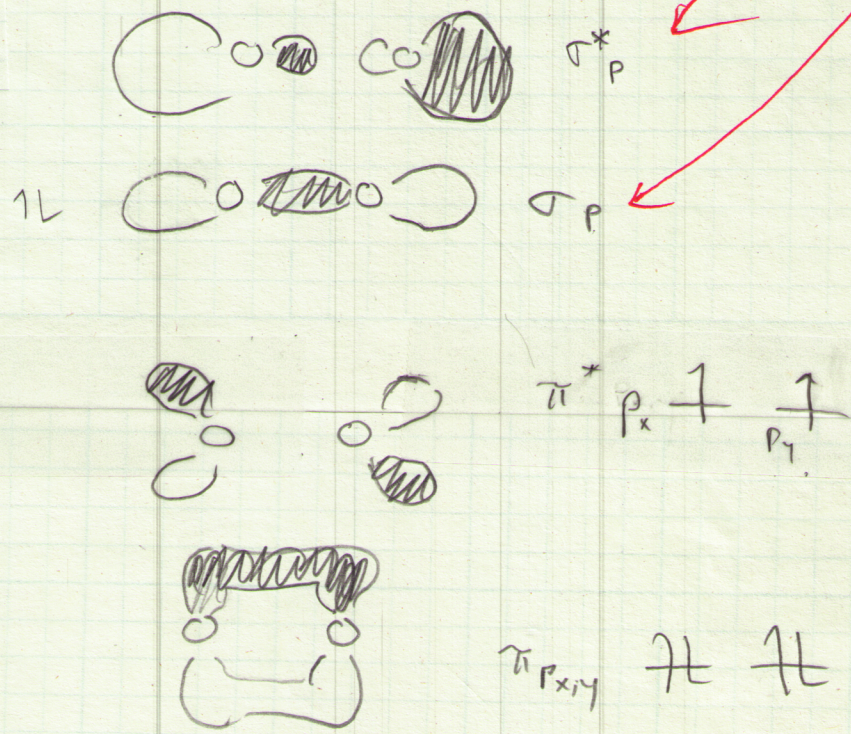
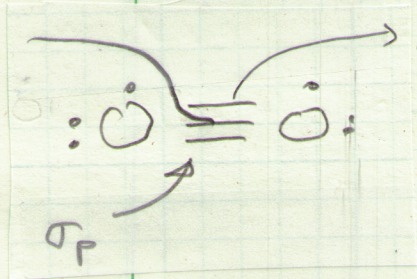
REL ENERGY



MO



$\frac{1}{2} \pi$ bond



why $\frac{1}{2} \pi$ bonds?
 1 antibonding e^-
 +
 2 bonding e^-
 "1 bonding e^- "

$\frac{1}{2} \pi$ bond
 equivalent

Bond order = 2
 val e^- lone pair e^-
 $\frac{12 - 8}{2} = \frac{4}{2} = 2$