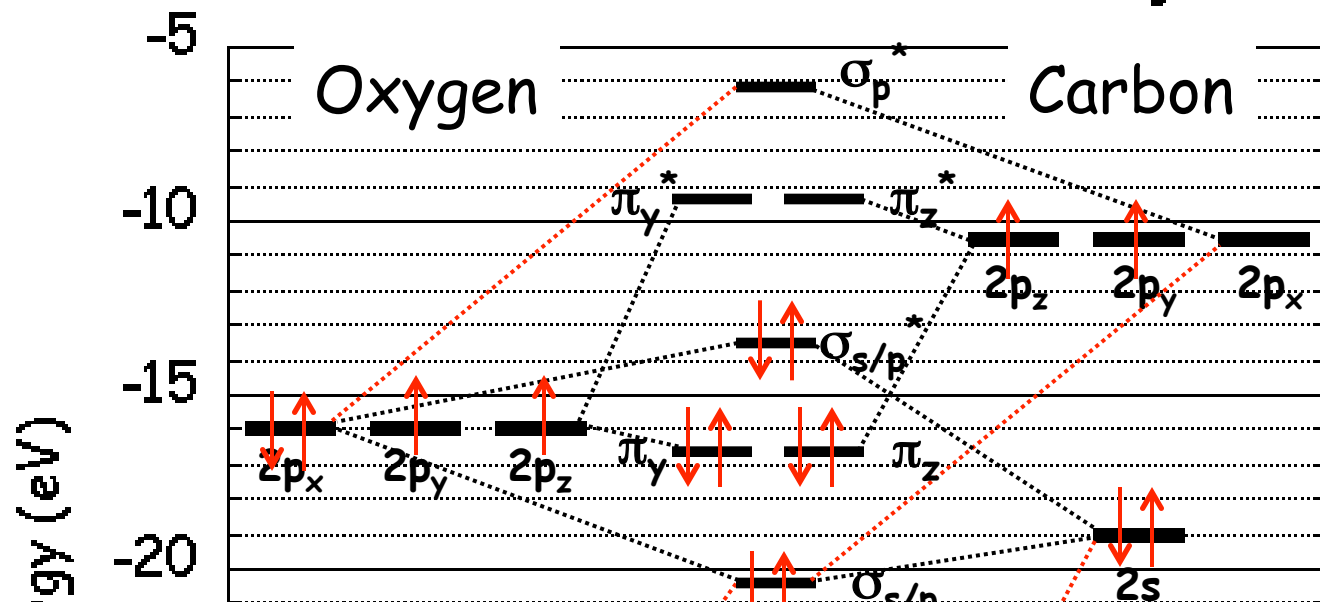


# The Nucleophilic and Electrophilic Sites in CO

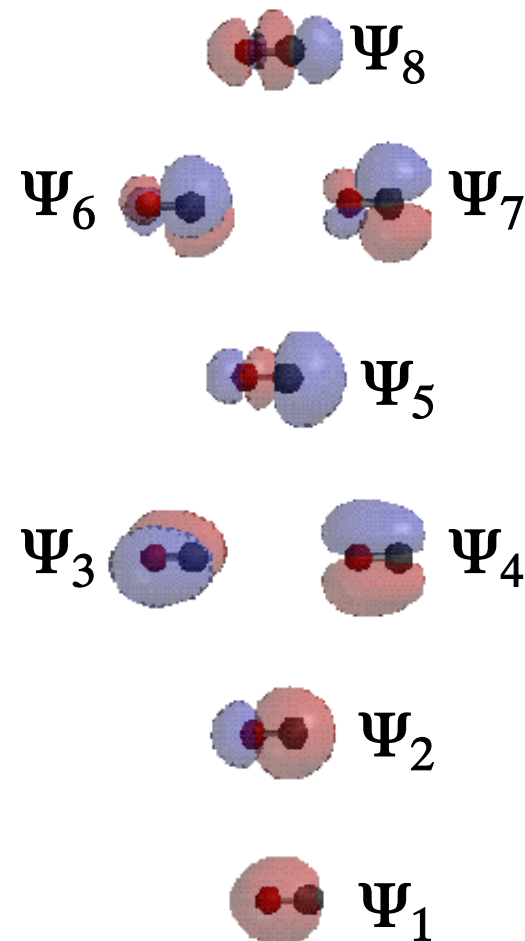
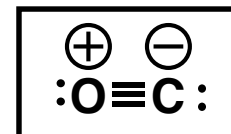
Carbon Monoxide Orbital Interaction Diagram



Energy (eV)

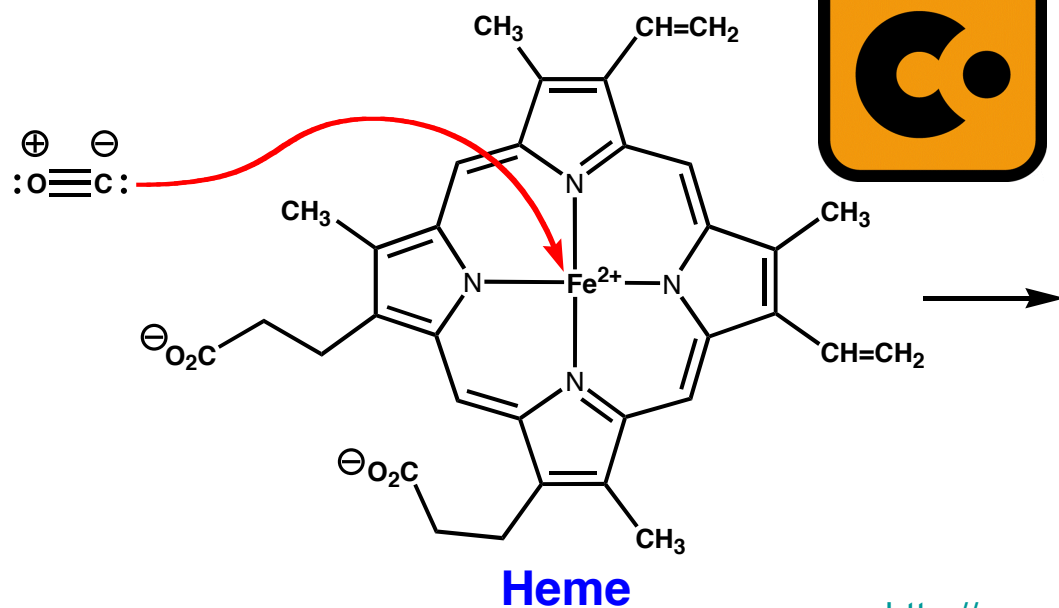
Nucleophilic site: use the energy diagram to locate the highest occupied MO = HOMO ( $\sigma_{s/p}^*$ ). Look at the corresponding orbital ( $\Psi_5$  image). On which atom does the largest share of this orbital reside?

Electrophilic site: use the energy diagram to locate the lowest unoccupied MO = LUMO ( $\pi^*$ ). Look at the corresponding orbital ( $\Psi_6$   $\Psi_7$  images). On which atom does the largest share of this orbital reside?

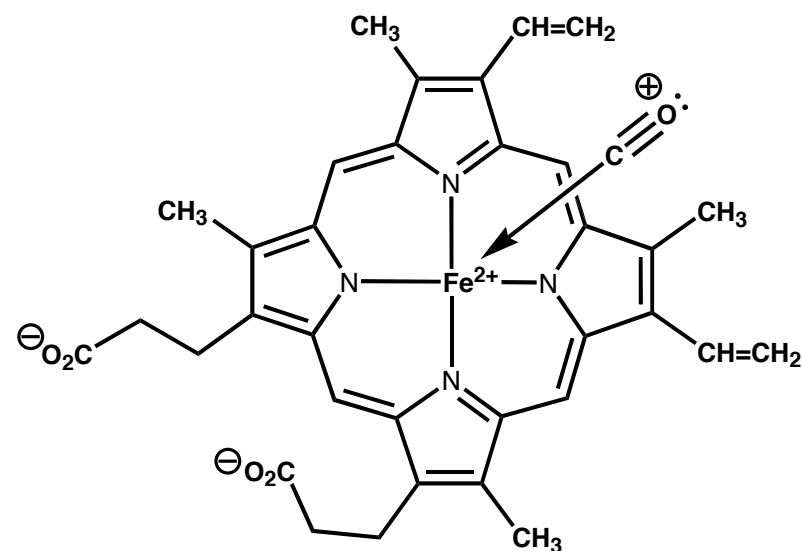


# Carbon Monoxide's HOMO and LUMO Define Its Reactivity

carbon monoxide as a nucleophile (HOMO)



Why carbon monoxide is poisonous.



<http://www.pdb.org/pdb/explore/jmol.do?structureId=1MZO>

carbon monoxide as a electrophile (LUMO)

