This Class

Finsh 5.1 Formation of Molecular Orbitals

5.2 Homonuclear Diatomic Molecules

5.3 Heteronuclear Diatomic Molecules

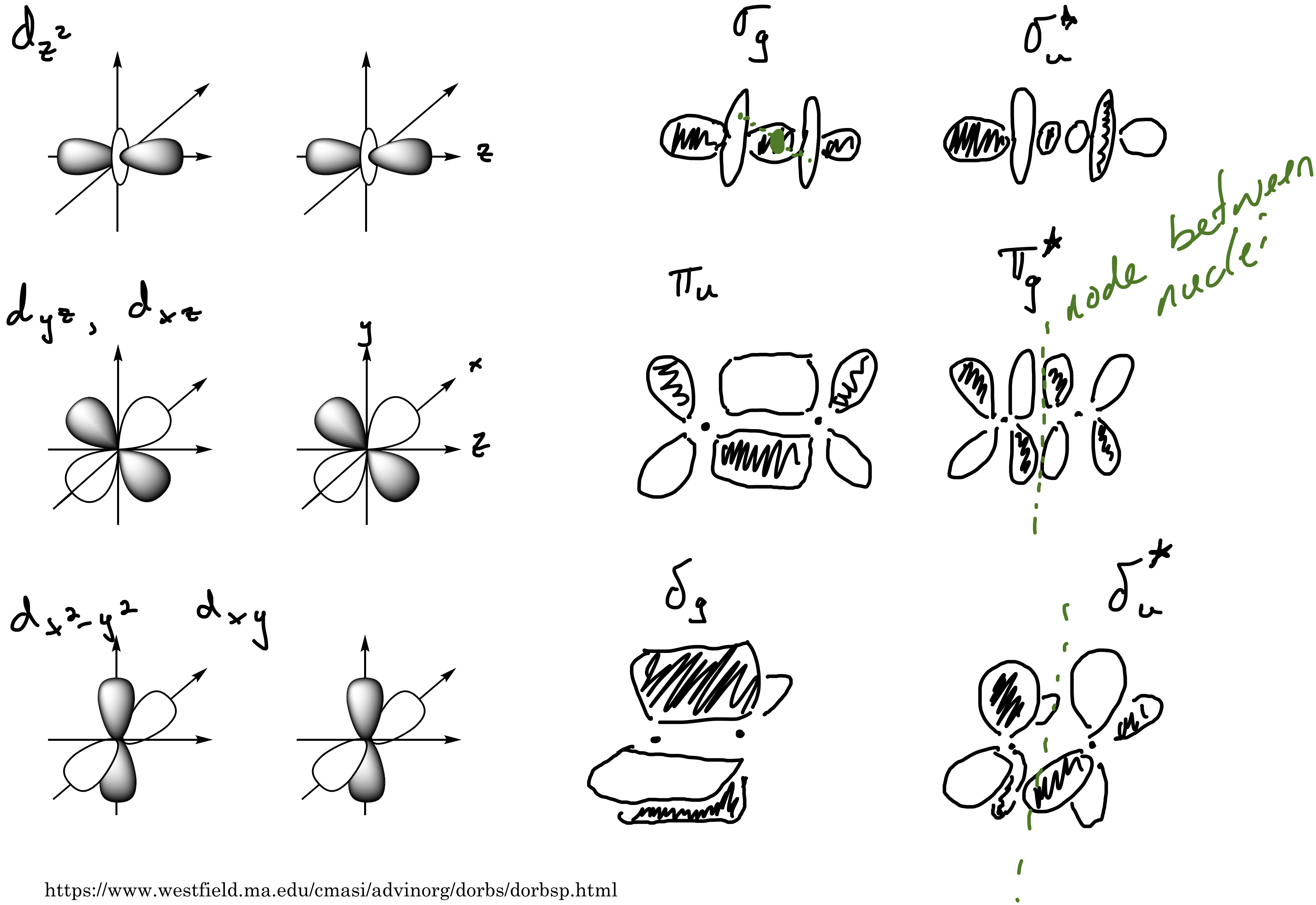
Next Class

5.3 Heteronuclear Diatomic Molecules

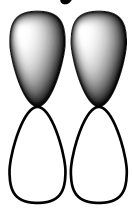
Orbital Mixing in Diatomic Molecules

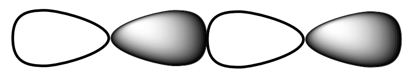
Heteronuclear Diatomic Molecules

Polyatomic molecules

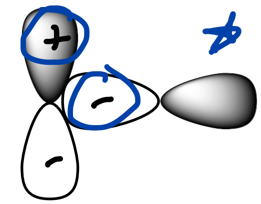


https://www.westfield.ma.edu/cmasi/advinorg/dorbs/dorbsp.html





not ok



lobes of the same sign or opposite sign interact

lobes that interact with both + & −

* when I add, the − and − constructively interfere but at the same time, the + and − destructively interfere. So no net interaction

Bonding - contructive interference ... increased volume between nuclei ... lower in E than AO's

Anitbonding - destructive interference ... node forms between higher in E than the AO's

Nonbonding - neither constructive nor destructive interference .... E is essentially the same as the AO's

"orphaned" orbitals - no symmetry match
- energy too different

three AO's interact to form 3 MO's
often the middle one is non bonding

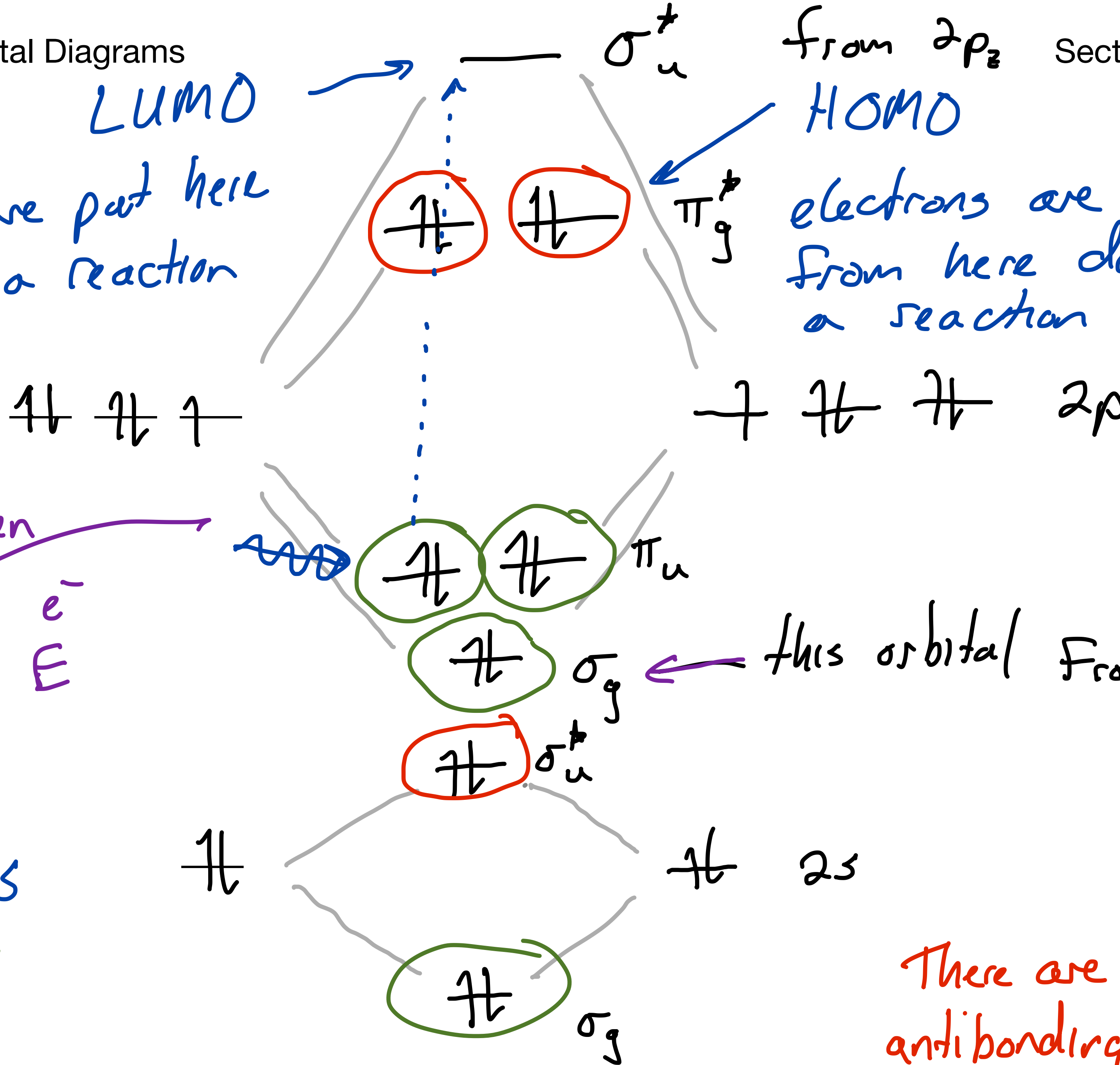
F_2

e^-'s are put here during a reaction

LUMO

HOMO

electrons are taken from here during a reaction



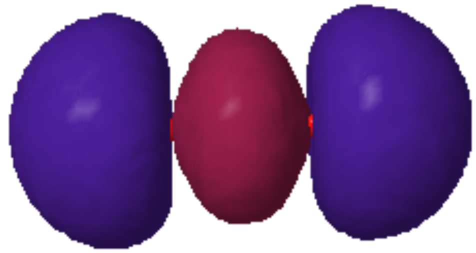
a photon can excite the e^- to a higher E orbital

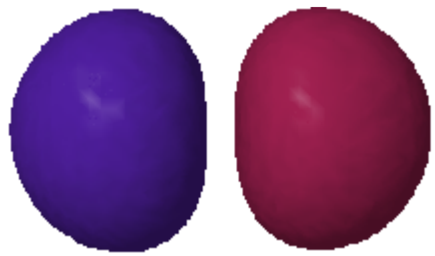
this orbital from $2p_z$

There are 8 bonding e^-

There are 6 antibonding e^-

$$BO = \frac{8-6}{2} = 1 \qquad \frac{7-7}{2}$$

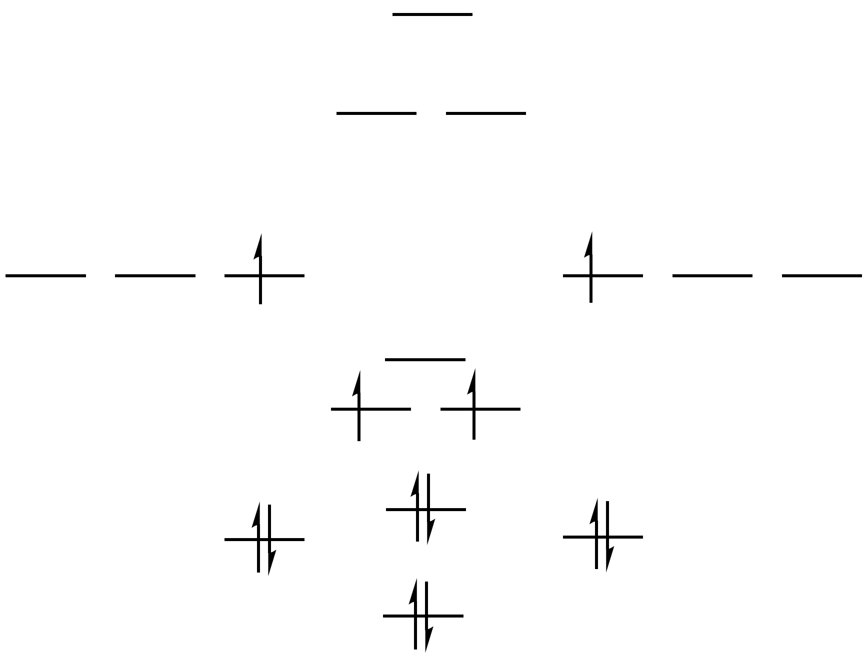


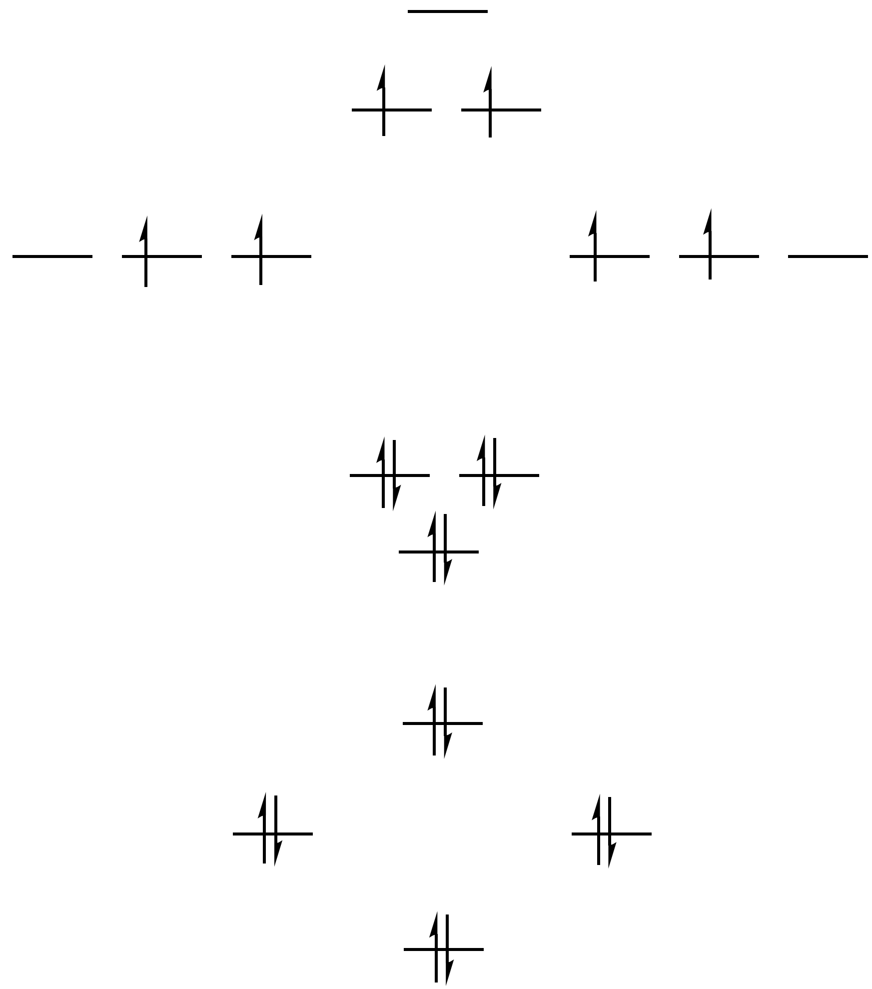


2s orbital

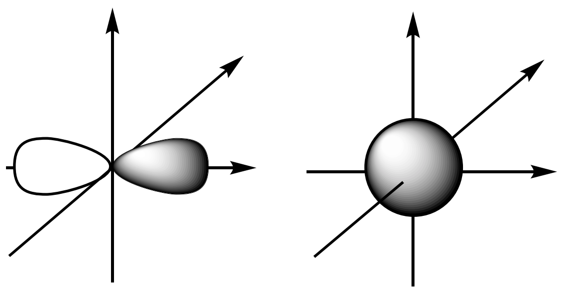
2s orbital

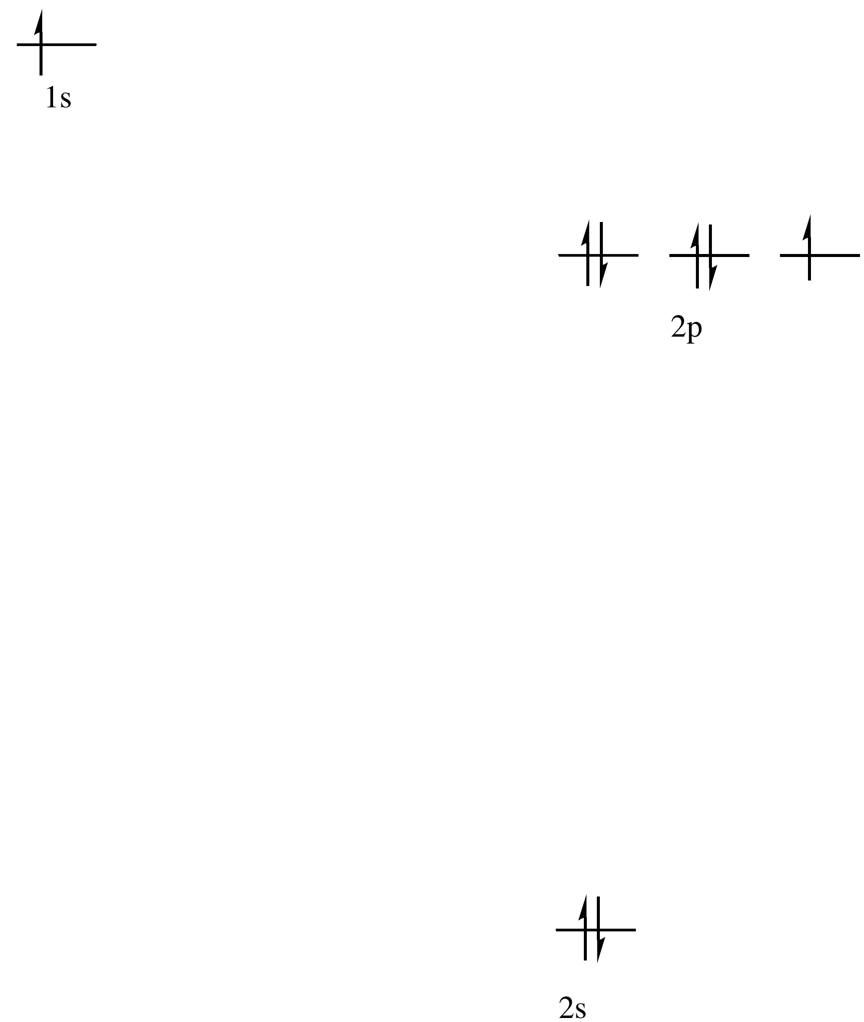
$$\Psi(\sigma_g(s)) = N[c_a\psi(2s_a) + c_b\psi(2s_b)]$$





$$\Psi(\sigma_g(s)) = N[c_a\psi(2s_a) + c_b\psi(2s_b) + c_c\psi(2p_a) + c_d\psi(2p_b)]$$




1s
2p
2s

Heteronuclear Diatomic Molecules: CO