This Class

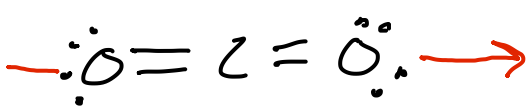
5.4 Polyatomic Molecules

Next Class

Chap 6 Acid and Bases

1. Draw a Lewis Structure.
2. Use VSEPR rules to determine geometry
3. Determine the Pt. Group for the molecule
4. Determine the symmetry of the SALC's for the orbitals on the atoms at the periphery
   A. Find reducible representations for each set
      1. Just H atoms just SALC's made from 1s
      2. Second row elements SALCs from 2s, and 2p's
         2px's interact with 2px
         2py with 2py
         2pz with 2pz
   B. Find irreducible representations for each set of SALC's
5. Read off the symmetry of the orbitals on the atom at the center of the molecule
   - Look in the "function" colums x for px, y for py, and z for pz
   - Look int he second function column for xy, xz, yz, z^2, and X^2+y^2
   - s orbitals are always symmetrical with respect to every symmetry operation
      1's all. The way across
6. Match up symmetry appropriate orbitals and make reasonable predictions about interactions
   - orbitals close in E interact strongly
   - orbitals far away in E interact weakly

Pt. Grp.?



$D_{\infty h}$

infinity ?

C_{∞}

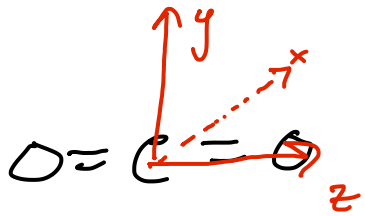
D_{2h} as a stand in

C_{2v} D_{3h}

axes of rotation

principle axis is C_2

principle axis is C_3



Symmetry of O's 2s SALCs?

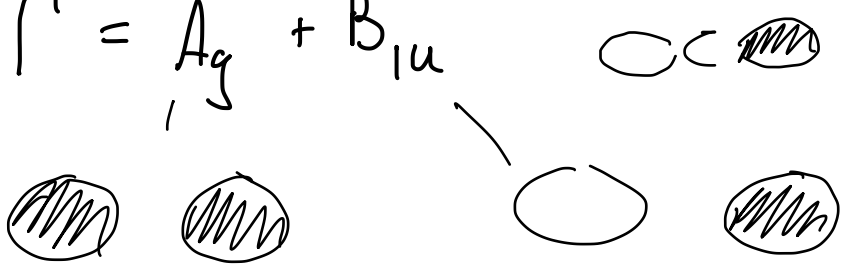
D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma_h(xy)$	$\sigma_d(xz)$	$\sigma_d(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	xy
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y	xz
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	yz
A_u	1	1	1	1	-1	-1	-1	-1		
B_{1u}	1	1	-1	-1	-1	-1	1	1	z	
B_{2u}	1	-1	1	-1	-1	1	-1	1	y	
B_{3u}	1	-1	-1	1	-1	1	1	-1	x	

Γ 2 2 0 0 0 0 2 2

both O atoms changed position

looked for something to add to Ag to "cancel out" the middle 4 1's

$\Gamma = A_g + B_{1u}$



Symmetry for O's 2p SALCs?

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma_h(xy)$	$\sigma_d(xz)$	$\sigma_d(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	xy
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y	xz
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	yz
A_u	1	1	1	1	-1	-1	-1	-1		
B_{1u}	1	1	-1	-1	-1	-1	1	1	z	
B_{2u}	1	-1	1	-1	-1	1	-1	1	y	
B_{3u}	1	-1	-1	1	-1	1	1	-1	x	

1st row Γ_{2p_x} 2 −2 0 0 0 0 2 −2 not A_g A_u B_{1g}

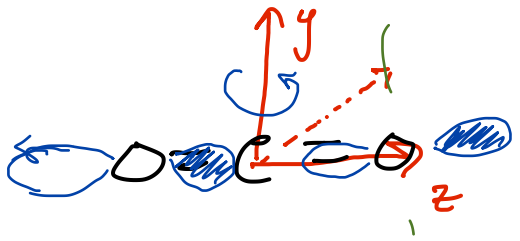
$B_{2g} + B_{3u}$

2nd row Γ_{2p_y} 2 −2 0 0 0 0 −2 2 not A_g A_u B_{1u}

$B_{3g} + B_{2u}$

3rd row $2p_z$ 2 2 0 0 0 0 2 2

$A_g + B_{1u}$



Symmetry matches with C's orbitals?

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma_h(xy)$	$\sigma_d(xz)$	$\sigma_d(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	xy
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y	xz
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	yz
A_u	1	1	1	1	-1	-1	-1	-1		
B_{1u}	1	1	-1	-1	-1	-1	1	1	z	
B_{2u}	1	-1	1	-1	-1	1	-1	1	y	
B_{3u}	1	-1	-1	1	-1	1	1	-1	x	

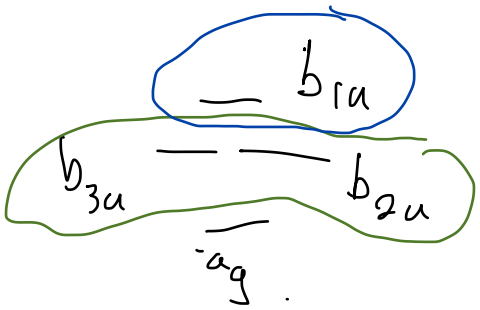
C $2p_x$? B_{3u}

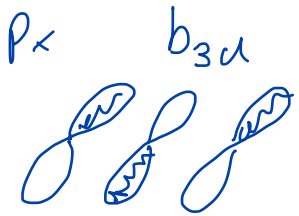
C's $2p_y$ is B_{2u}

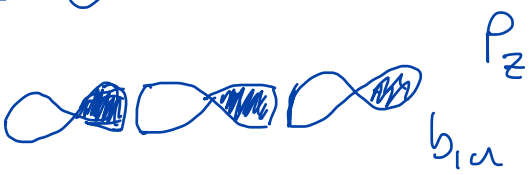
C's $2p_z$ is B_{1u}

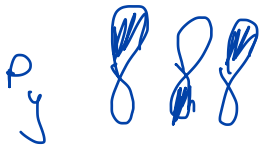
C's 2s ? A_g

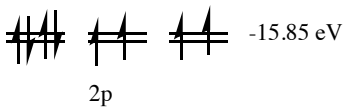
MO Diagram for CO_2

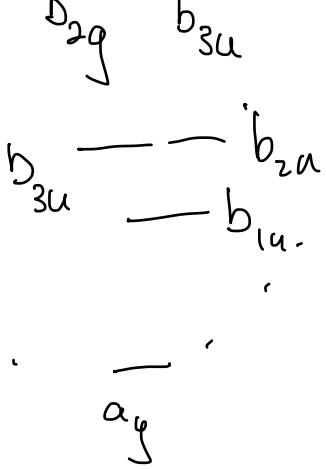


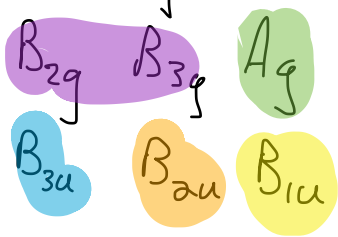






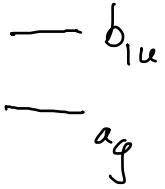






no symmetry match

so non bonding



C

CO_2

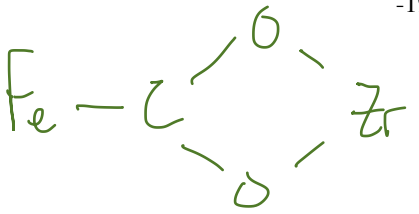
-32.38 eV

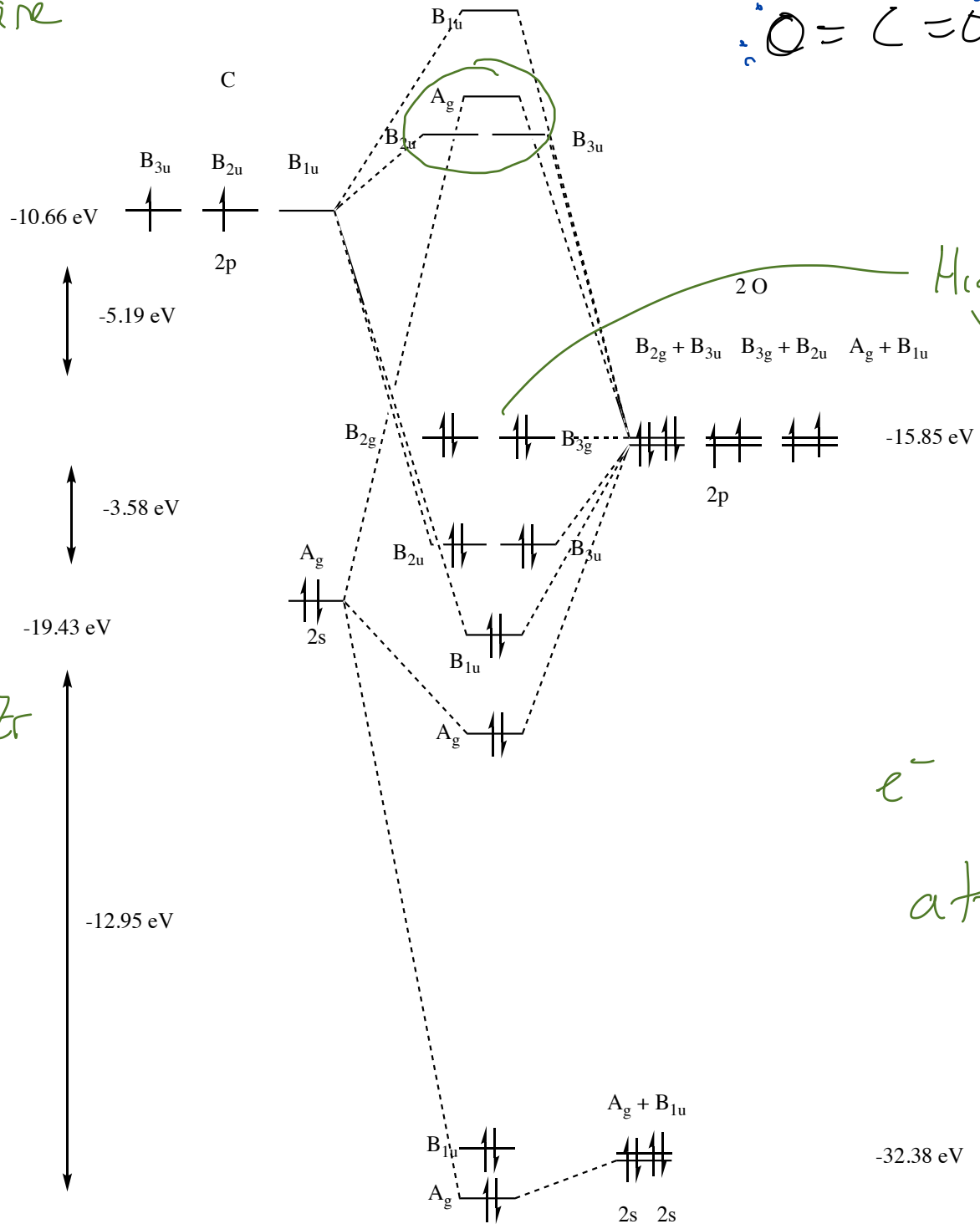
too far away in E to interact strongly

weak interaction

LUMO's are C based

e⁻ rich atom attack C





Highest Occupied Molecular Orbitals are O atom based

e⁻ poor atom attack O