(21) **Today**

5.4 Polyatomic Molecules

Next Class (22)

Chap 6 Acid-Base and Donor-Acceptor Chemistry

(23) **Second Class from Today**

Chap 6 Acid-Base and Donor-Acceptor Chemistry

Third Class from Today (24)

Chap 6 Acid-Base and Donor-Acceptor Chemistry

Test 2 postponed to 11/6

Office hours postponed to 12:30 to 1:15

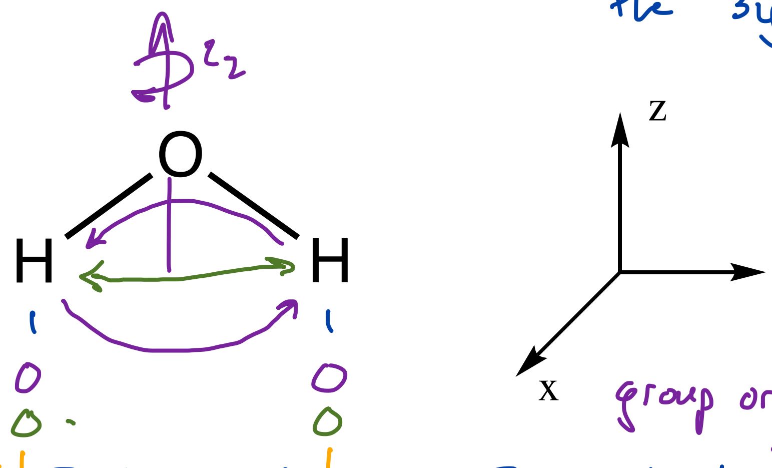
~~Introduce MOs (s, p, d orbital interactions)~~

~~Diatomic Molecules and Orbital Mixing~~

~~Heteronuclear Diatomic Molecules~~

~~Polya~~tomic molecules

We use character tables to determine the symmetry of the SALC's formed from H's 1s orbitals



the reducible representation for the group orbitals made from H's 1s's

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz
Γ	2	0	0	2		

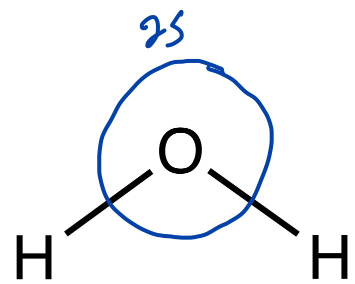
$\Gamma = A_1 + B_2$

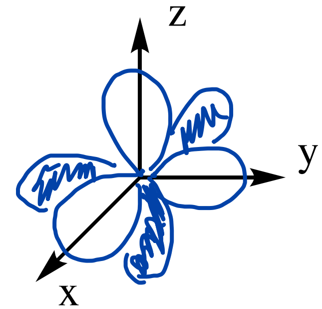
1. Find point group for molecule
2. Find reducible representation for orbitals that make up the SALC
3. Find irreducible representations that combine to form the reducible representation

2 1s's ⟶ 2 SALC's with A_1 + B_2

the back of the 1s orbital is reflected to the front, so there is no change in position since 1s is ⊕ phase all the way around there is no change in sign

For the central atom use the matching functions





C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

$B_1 = \Gamma \quad 1 \quad -1 \quad 1 \quad -1$

$2p_z = z = A_1$

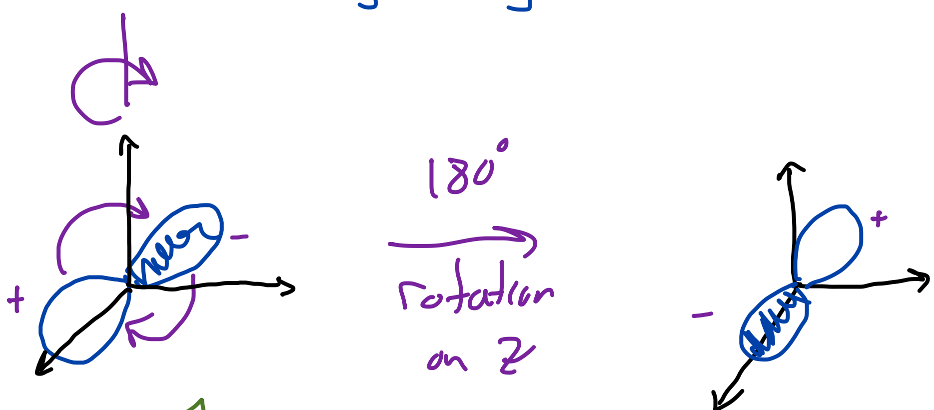
$2p_y = y = B_2$

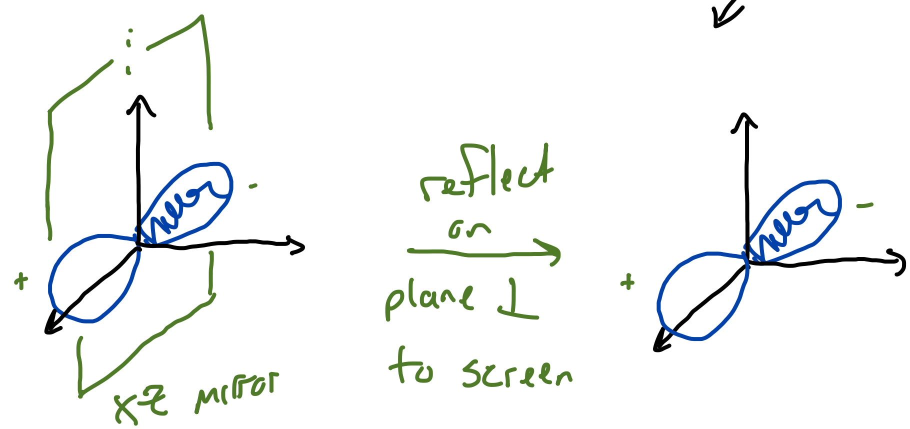
$2p_x = x = B_1$

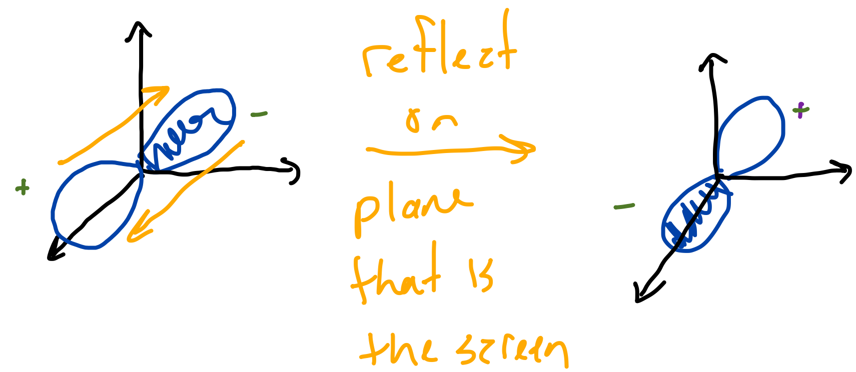
$2s$ = spherecally symmetry = A_1

= all χ are 1's

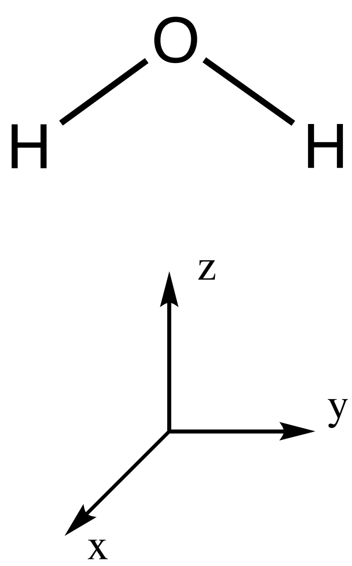
what is the symmetry of the $2p_x$ orbital

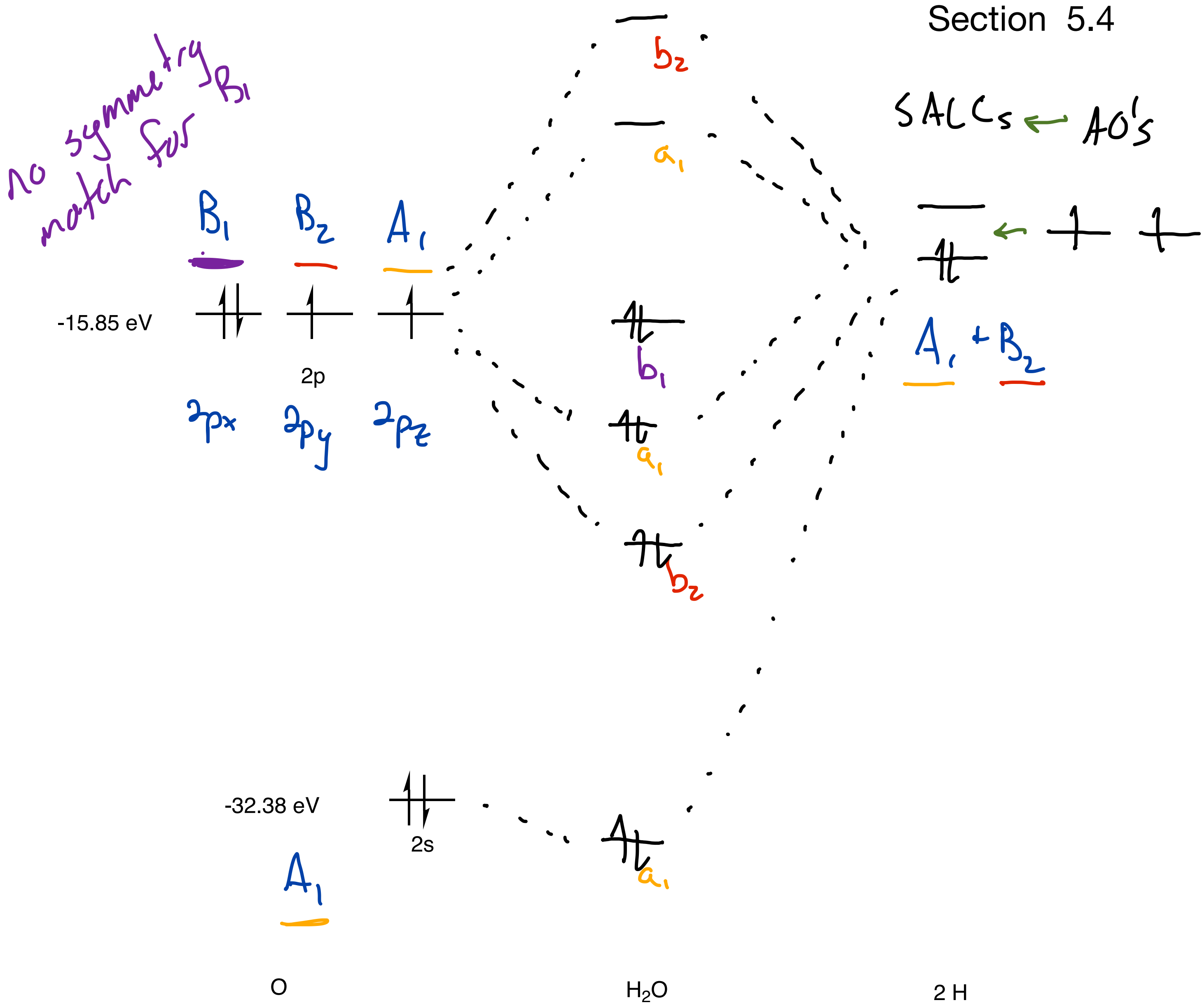




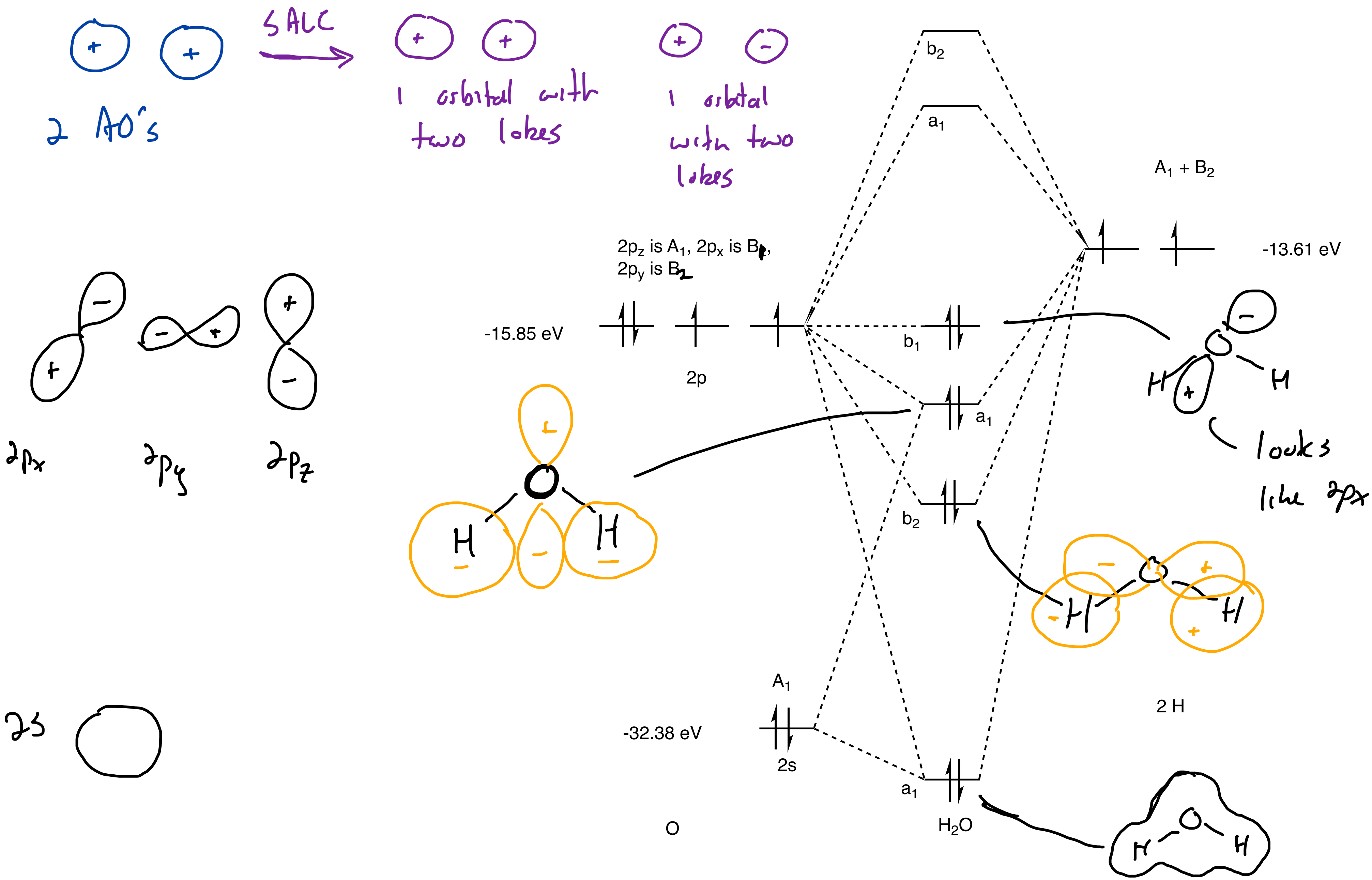


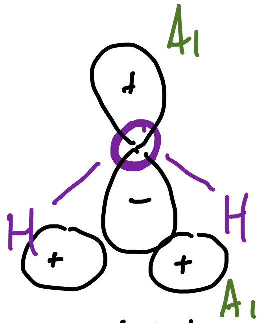
MO Diagram for H_2O





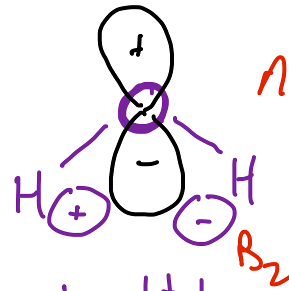
Interpreting the MO Diagram for H_2O





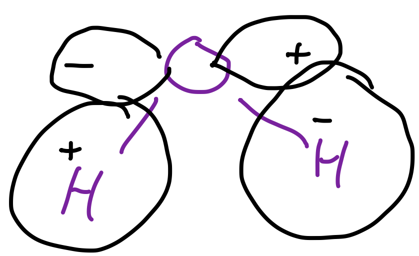
1 orbital with two lobes

this is fine ⊖ of $2p_z$ only interacts with ⊕ of group orbital



1 orbital with two lobes

no net interaction the ⊖ of the $2p_z$ interacts with the ⊕ + ⊖ of the group orbital



adding would cause destructive interference

subtracting would cause constructive interference

(1) Lewis Structure

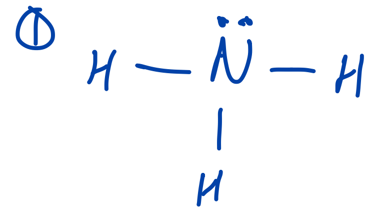
(2) Use VSEPR Rules to Determine the Shape

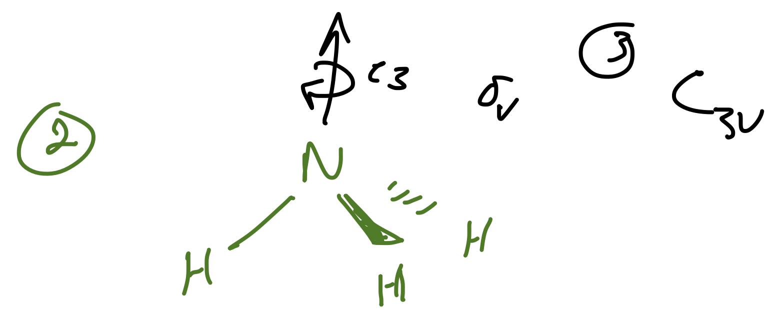
(3) Find Point Group

(4) Determine Symmetry of Symmetry Adapted Linear Combinations of the three 1s orbitals on the there H atoms

(5) Find Orbitals on N with Matching Symmetry

Add and Subtract Orbitals to From Molecular Orbitals





C_{3v}	E	2 C_3	3 σ_v		
A_1	1	1	1	z 5	$x^2 + y^2$, z^2
A_2	1	1	-1	R_z	
E	2	-1	0	(x, y), (R_x, R_y)	($x^2 - y^2$, xy), (xz, yz)
Γ	3	0	1		

c)

N 2s A_1

N 2p_z A_1

N 2p_x, 2p_y = E

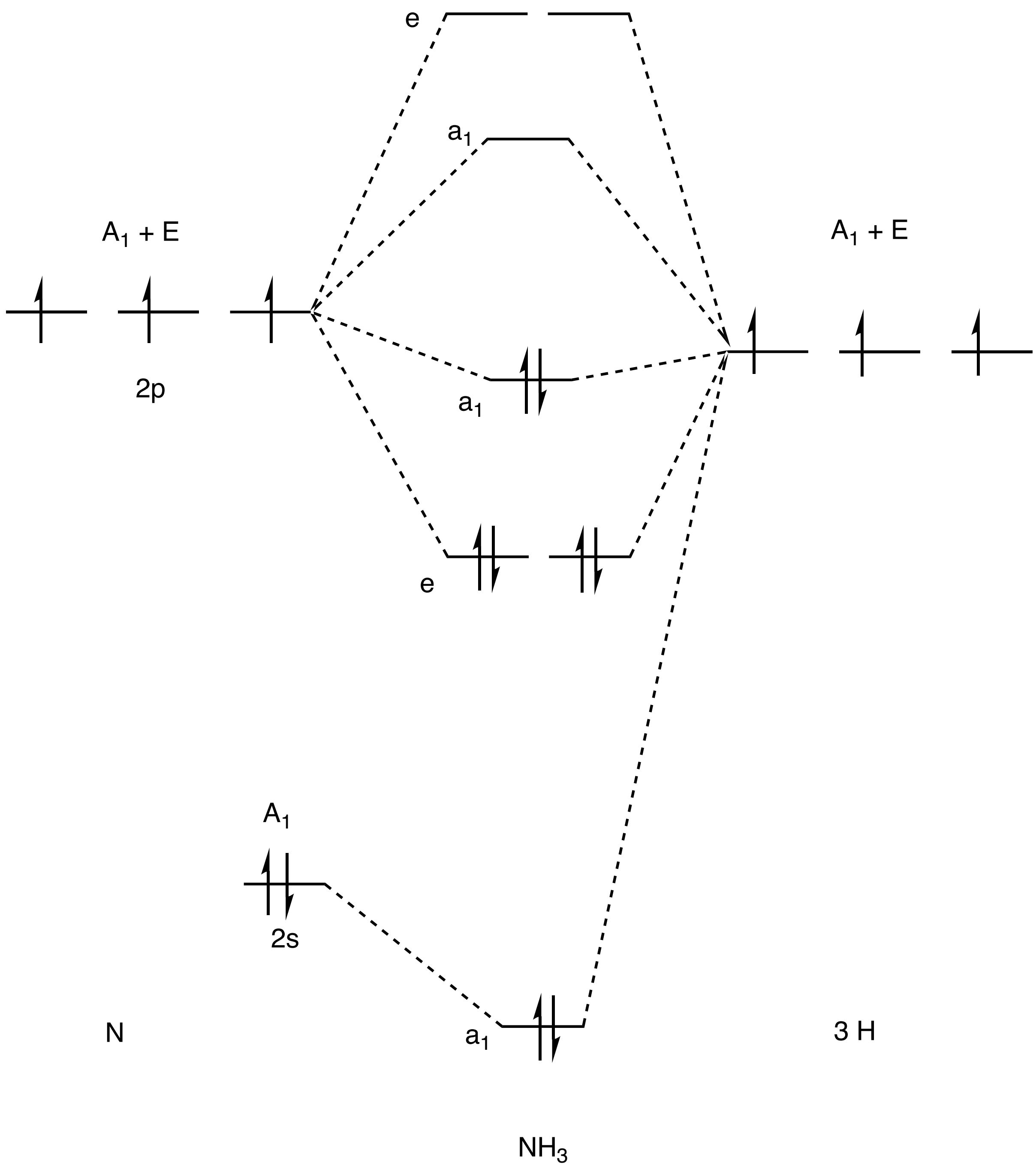
$\Gamma = A_1 + E$ (by inspection)

$\#A1 = \frac{1}{6}(1 \cdot 1 \cdot 3 + 2 \cdot 1 \cdot 0 + 3 \cdot 1 \cdot 1) = 1$

$\#A2 = \frac{1}{6}(1 \cdot 1 \cdot 3 + 2 \cdot 1 \cdot 0 + 3 \cdot -1 \cdot 1) = 0$

$\#E = \frac{1}{6}(1 \cdot 2 \cdot 3 + 2 \cdot -1 \cdot 0 + 3 \cdot 0 \cdot 1) = 1$

(terms: 3, 0, 3; 3, 0, −3; 6, 0, 0) } by linear algebra


e
a1
A1 + E
2p
a1
A1 + E
e
A1
2s
N
a1
3 H
NH3