

(17) Today

5.4 Polyatomic Molecules

Next Class (18)

Chap 6 Acid-Base and Donor-Acceptor
Chemistry

(19) Second Class from Today

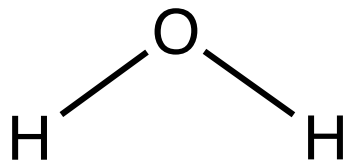
Chap 6 Acid-Base and Donor-Acceptor
Chemistry

Third Class from Today (20)

Chap 6 Acid-Base and Donor-Acceptor
Chemistry

Office Hours moved from 12:20 to 1:20 to 3:00 to 4:00 for the foreseeable future

Rework Test 1 and hand in on Friday, October 17. Rework means that you should, on a separate piece of paper, write a more complete answer for any question that you did not received full credit for. I do NOT need the test back.

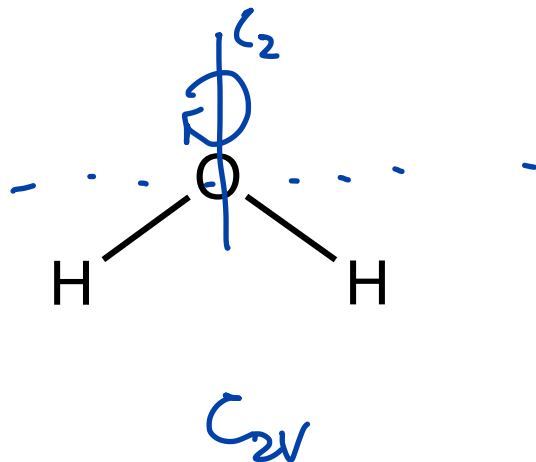


How do the $2s$ + $2p$ orbitals on O interact with the $1s$ orbitals on H? symmetry of the molecule determines orbital interactions

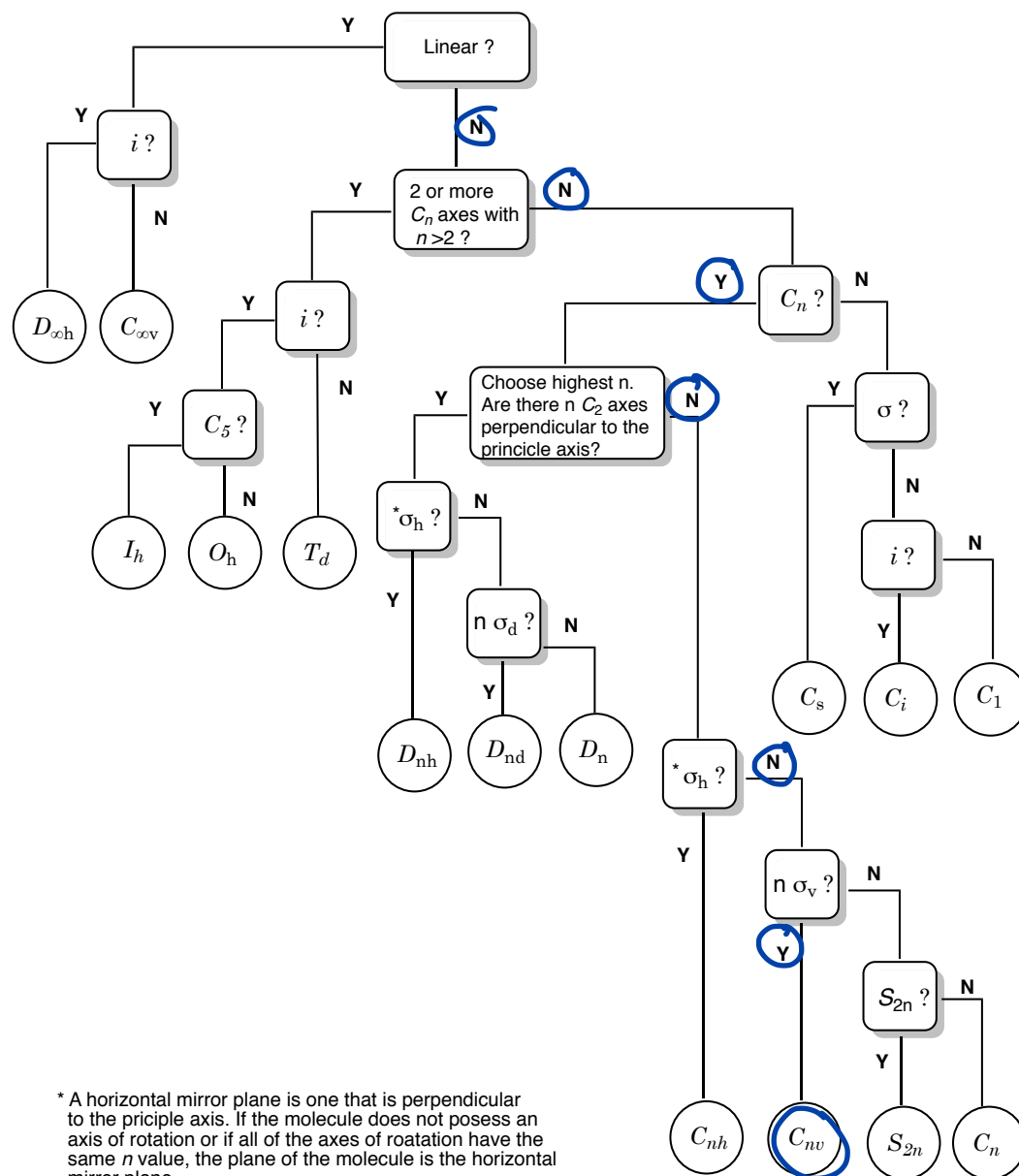
Symmetry Adapted Linear Combinations of orbitals on peripheral atoms

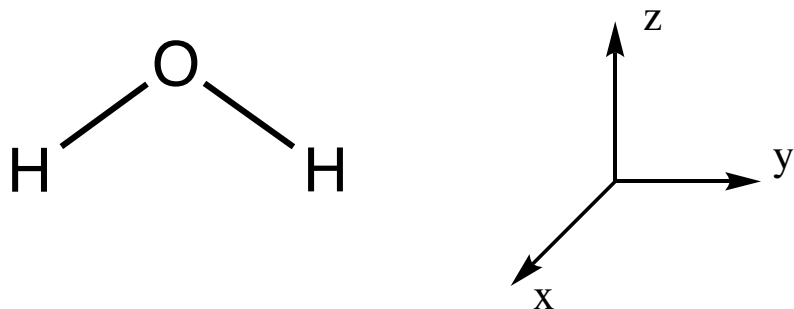
H's $1s$ orbitals will be treated as a group or a SALC 2 $1s$ orbitals will be combined to form 2 SALC's + those 2 SALC's will interact with symmetry appropriate orbitals on O

MO Diagram for H₂O



Section 5.4





What is the symmetry of the orbitals on the central atom

O's 2s A_1 s orbital on central atom is always the irreducible representation with all ones

$2p_x$ B_1
 $2p_y$ B_2
 $2p_z$ A_1

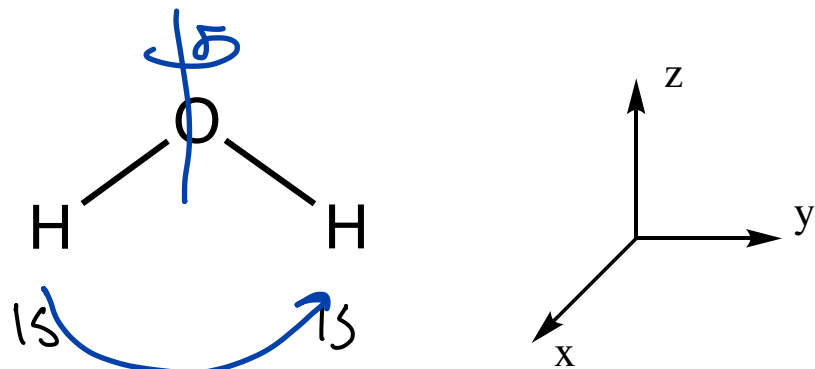
these are read from the function column

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

MO Diagram for H₂O: SALCs

Section 5.4

Find the reducible representation for the SALCs



before

1s_b

1s_a

1s_b

1s_a

1s_a

1s_b

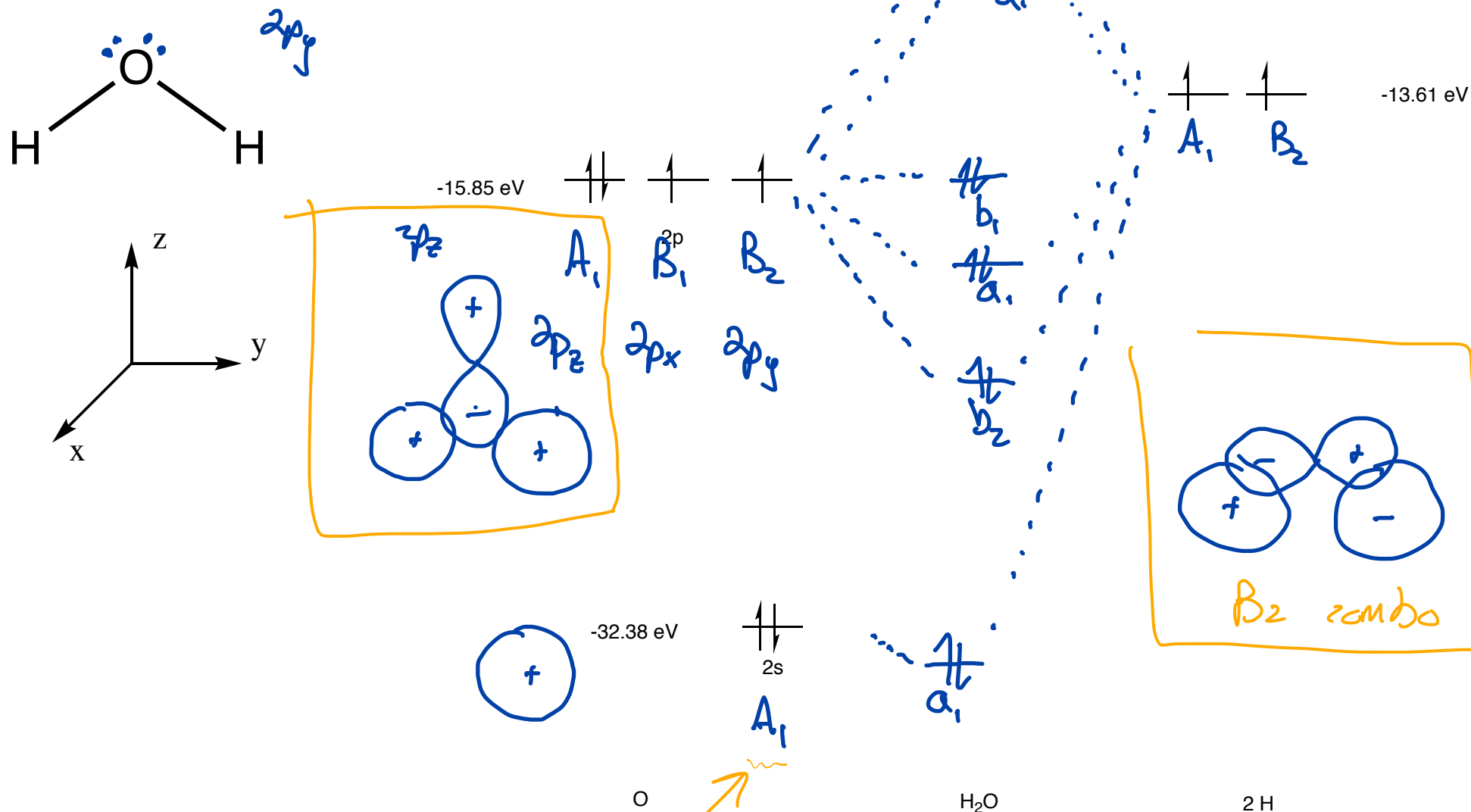
$$\Gamma = 2A_1 + B_2$$

C _{2v}	E	C ₂	σ _v (xz)	σ _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

one SALC with A₁ symmetry
 one SALC with B₂ symmetry
 both SALCs stretch over both H atom

MO Diagram for H₂O

Section 5.4



weak interaction with A_1 SALC

Polyatomic Molecules: NH_3

Section 5.4

① Lewis Structure

↓

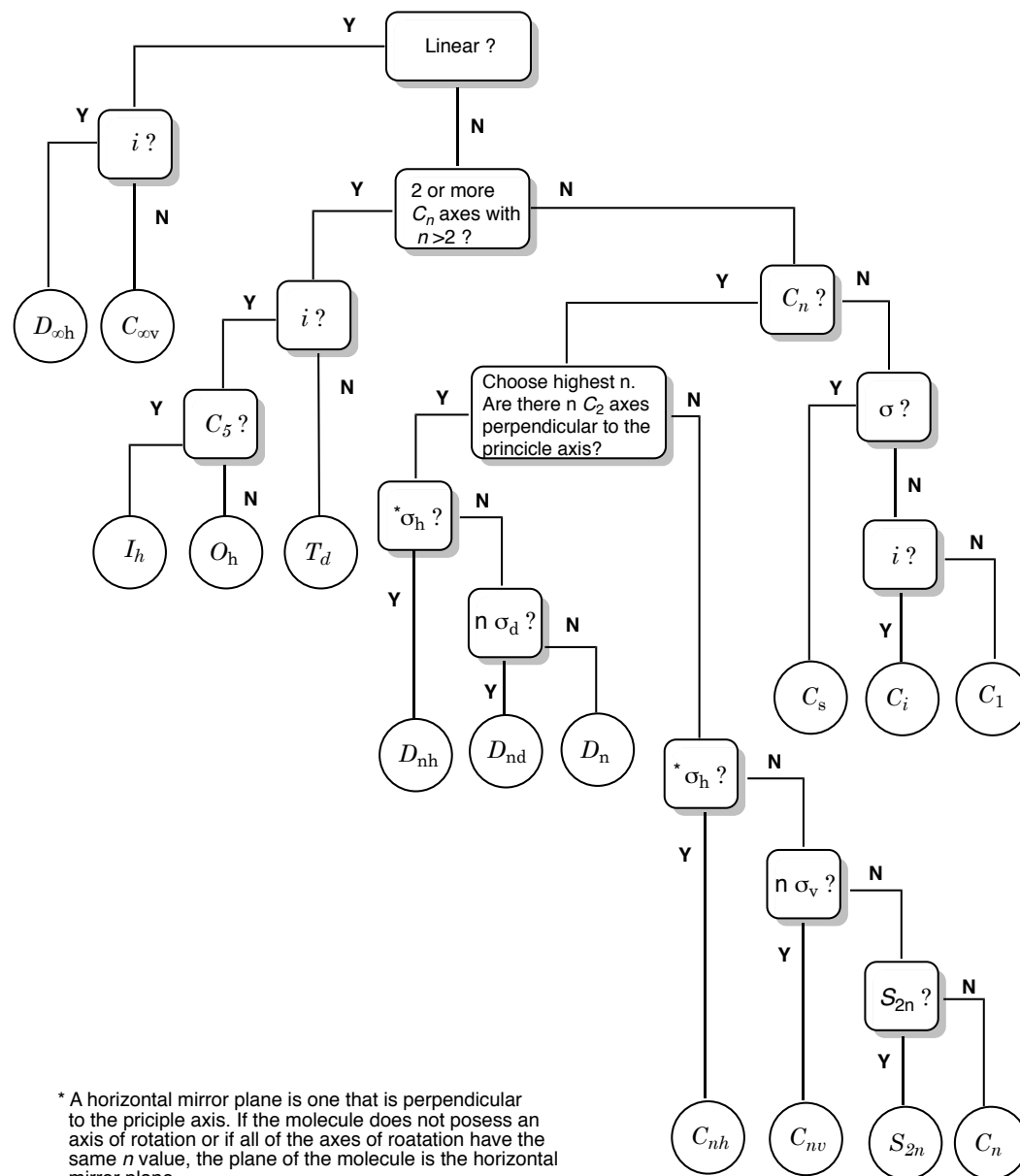
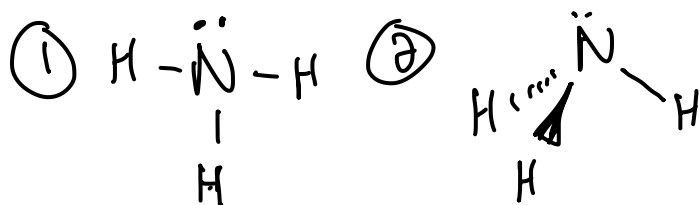
Use VSEPR Rules to Determine the Shape

Find Point Group

Determine Symmetry of Symmetry Adapted Linear Combinations of the three 1s orbitals on the three H atoms

Find Orbitals on N with Matching Symmetry

Add and Subtract Orbitals to Form Molecular Orbitals

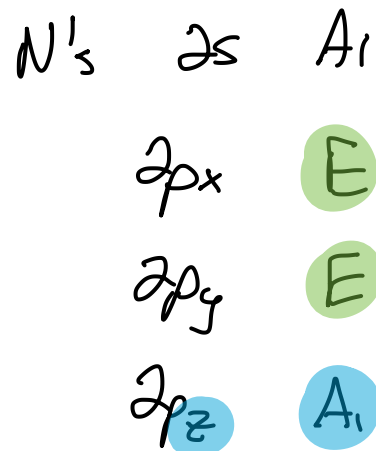
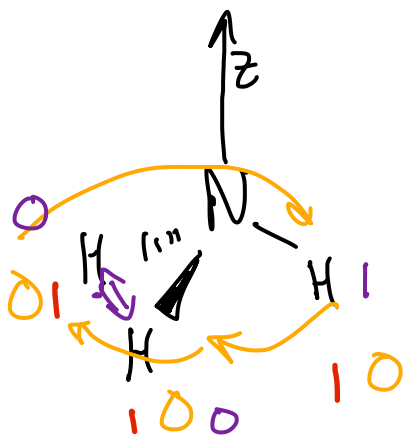


Polyatomic Molecules: NH₃

Section 5.4

C _{3v}	E	2 C ₃	3 σ _v		
A ₁	1	1	1	z	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)

$$\Gamma = 3 + 0 + 1 = A_1 + E$$



E means doubly degenerate... 2 things (SALCs) with the same symmetry & energy
 or
 (2p_x, 2p_y)

