(16) **Today**

4.4 Uses of Character Tables

Next Class (17)

5.1 Formation of Molecular Orbitals

5.2 Homonuclear Diatomic Molecules

(18) **Second Class from Today**

5.2 Homonuclear Diatomic Molecules

5.3 Heteronuclear Diatomic Molecules

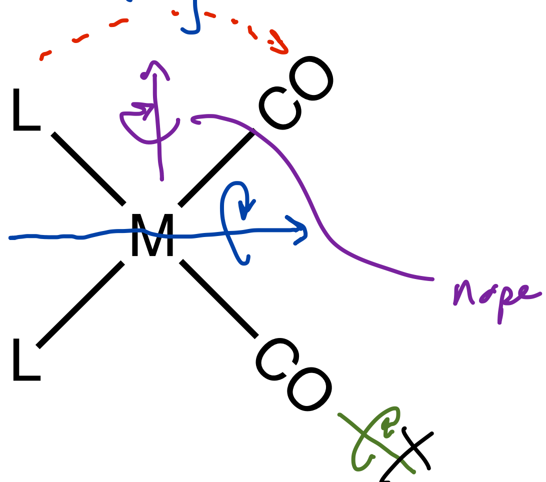
Third Class from Today (19)

5.3 Heteronuclear Diatomic Molecules

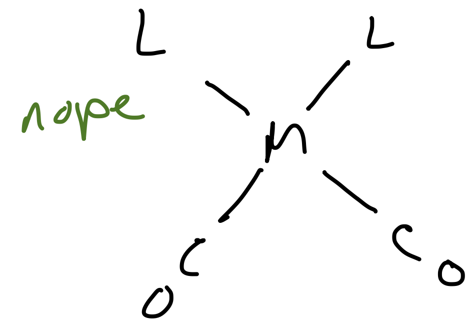
5.4 Polyatomic Molecules

Please rework test 1 and hand in on Monday, Oct 23

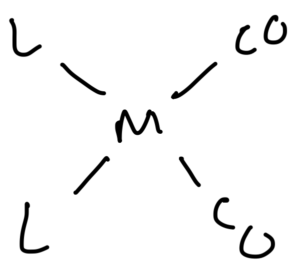
Tip: look along bonds
look along line the bisects bonds between identical atoms



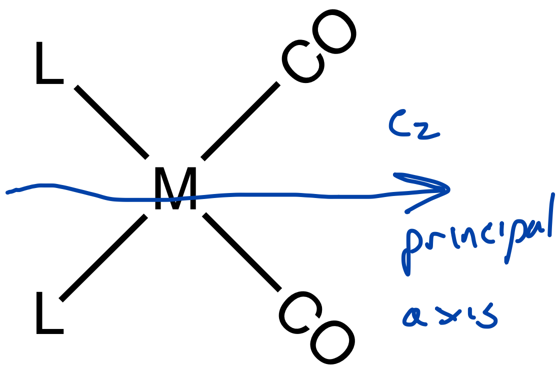
180° on L-M-CO line? ⇒



⇓ C_2 on line bisecting OC-M-CO angle? yep



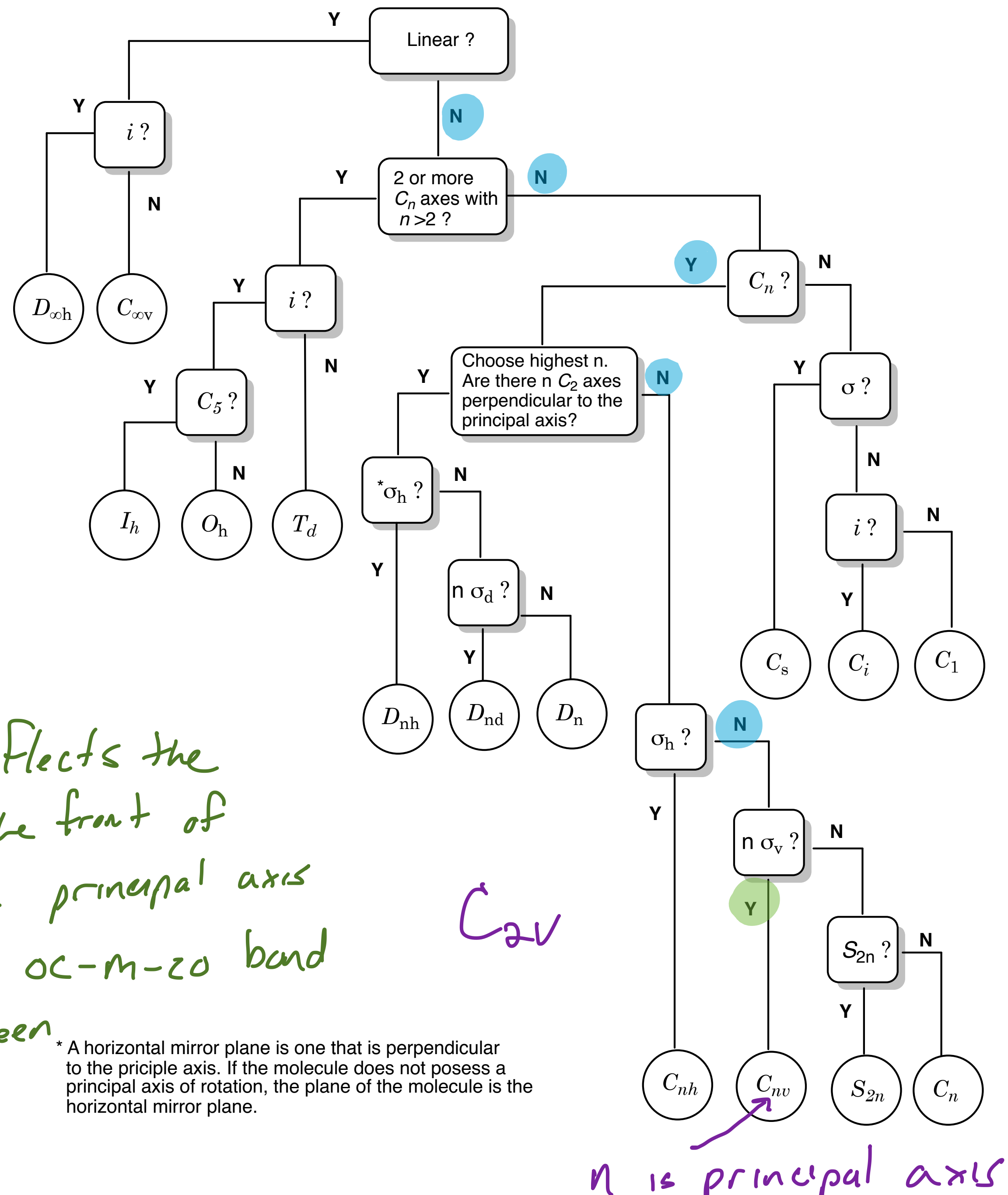
highest n is assigned as the principal axis & also as the z



mirror plane contains principal axis so is not a σ_h

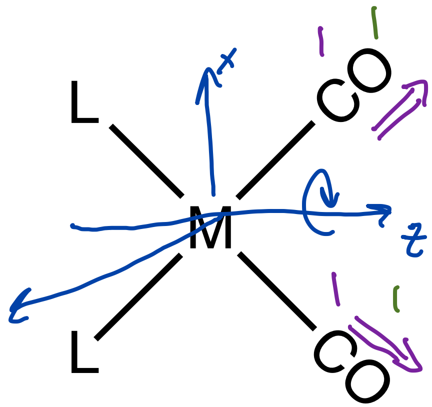
The plane of the screen reflects the back of the atoms to the front of the atoms + contains the principal axis

The plane that bisects the OC–M–CO bond angle and is ⊥ to the screen reflects top + bottom



* A horizontal mirror plane is one that is perpendicular to the priciple axis. If the molecule does not posess a principal axis of rotation, the plane of the molecule is the horizontal mirror plane.

Carbonyl Stretching Bands in Metal Compounds: Determine Reducible Representation



y axis comes out of the screen

E: do they change their position? no
do they change their direction? no
unchanged? yes 1 for each

C_2: they change their position 0 for each

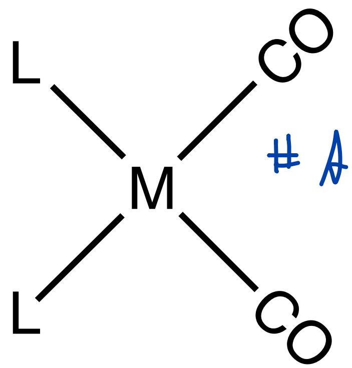
$\sigma_v(xz)$: they are unchange 1 for each

$\sigma(yz)$: they change their position 0 for each

plane of the screen

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	2	0		

Carbonyl Stretching Bands in Metal Compounds: Determine Irreducible Representations that Combine to Form Reducible Representation



$\# A_1 = \frac{1}{\text{order}}\left((1)(1)(2) + (1)(1)(0) + (1)(1)(2) + (1)(1)(0)\right)$

$= \frac{1}{4}(2+2)$

$\# A_1 = 1$

we can do this for each row or we can try by inspection ...

\# of operations in class

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	2	0		

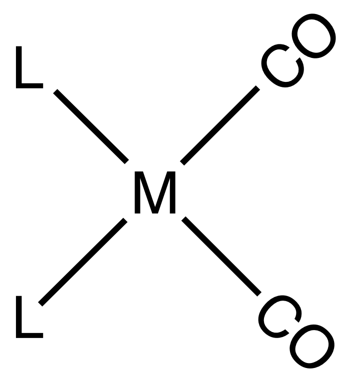
E C_2 σ_v

A_2? 2 2 (nope this need to sum to 0)

$A_2 + A_1$

$A_1 + B_1$ 2 0 2 0

$\Gamma = A_1 + B_1$



how many IR stretching bands should we see?

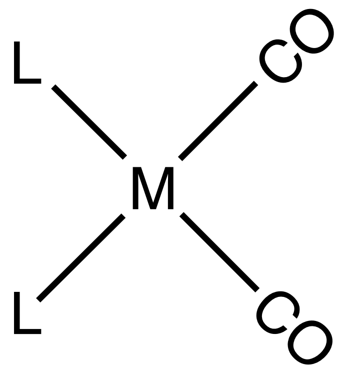
A_1 is a stretching mode that moves the atoms on z axis. Thus, dipole changes... IR active

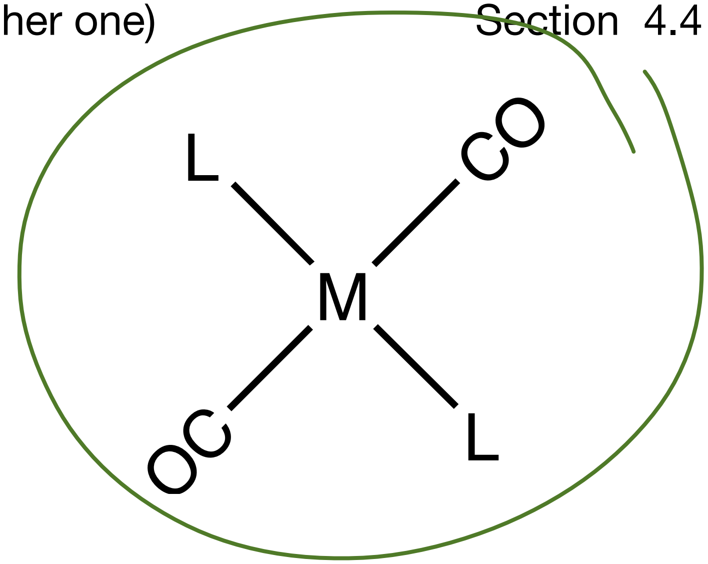
B_1 movement on x - yes IR active

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	2	0		

$\Gamma = A_1 + B_1$

2 CO stretching bands for C_{2v} square planar molecules with cis COs





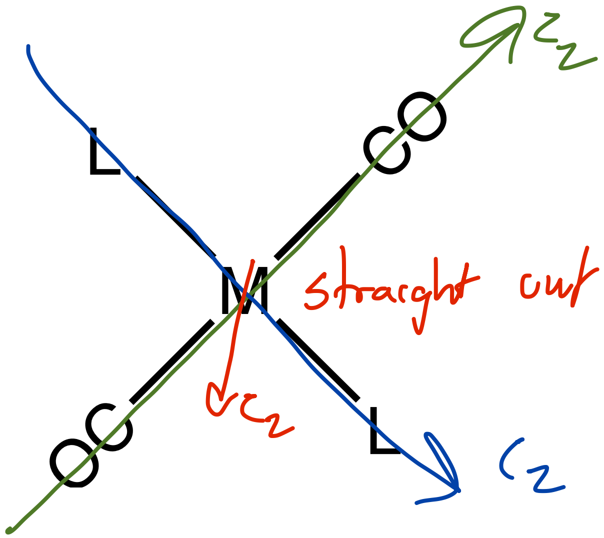
Find Rotational Axes and Assign x, y, and z Axes

Find Point Group

Determine Reducible Representation

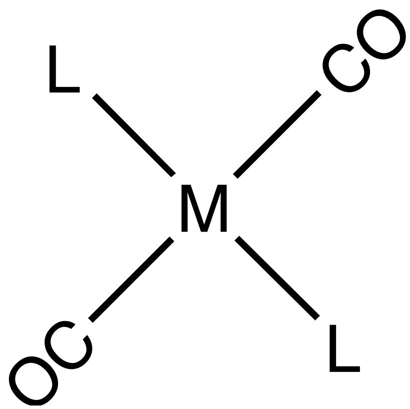
Determine Irreducible Representations that Combine to Form Reducible Representation

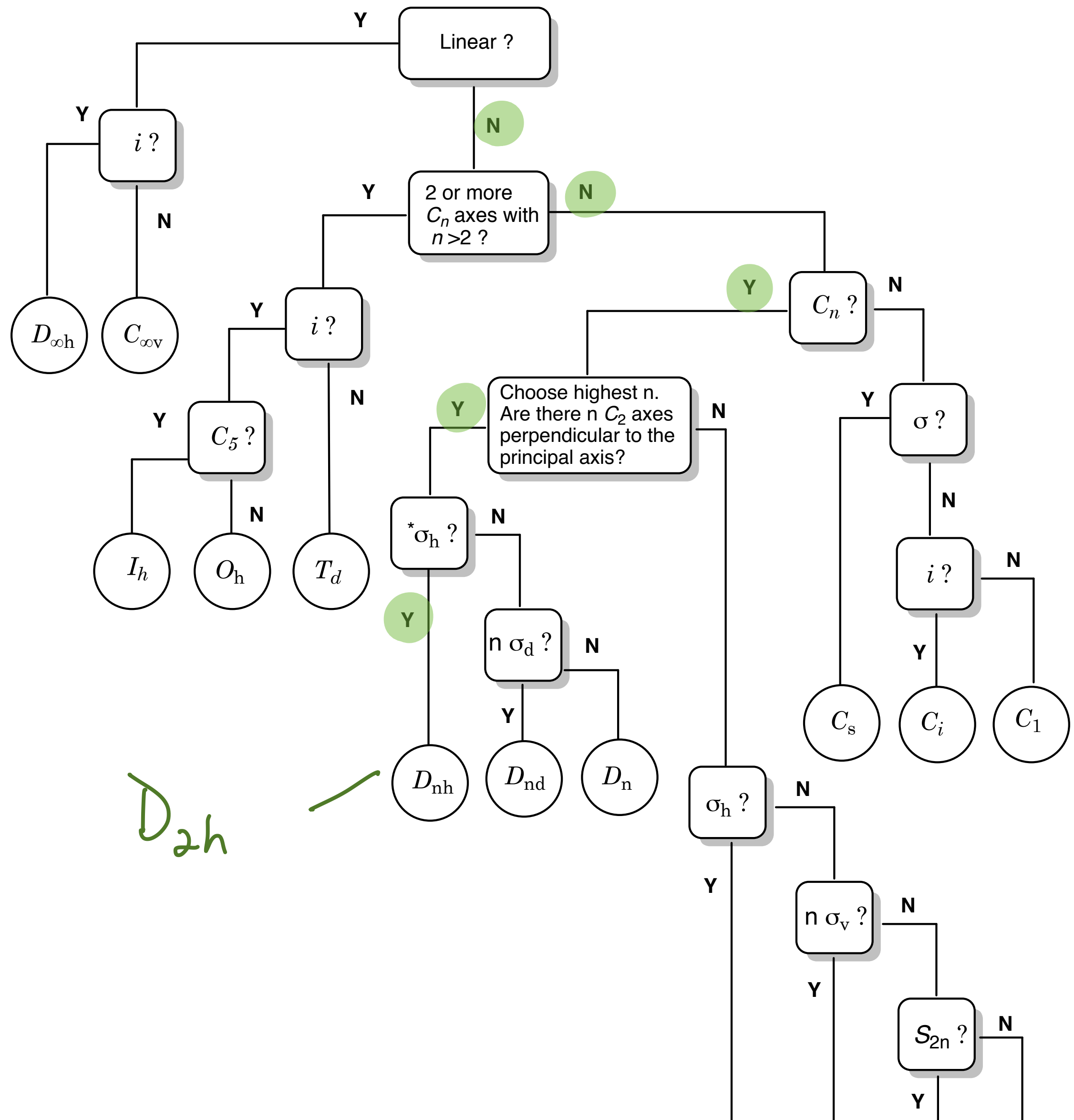
Analyze Results



Cn's

1 Find 3





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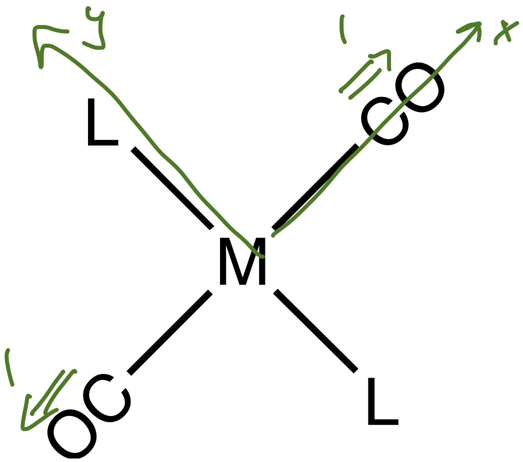
Carbonyl Stretching Bands in Metal Compounds (reducible representation) Section 4.4



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	0	0	2	0	2	2	0		

axis ⊥ to σ_h

$\Gamma = A_g + B_{3u}$ — moves dipole on x so IR active

(A_g) no movement of dipole on x, y, or z so not IR active