(12) **Today**

4.3 Character Tables

4.4 Uses of Character Tables

Next Class

Test 1 on Chap 1 through Chap 4 section 4.2 (symmetry operations and finding Point Groups)

(13) **Second Class from Today**

4.4 Uses of Character Tables

Third Class from Today (14)

Chapter 5: Molecular Orbital Theory

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	9	-1	3	1		

This summarizes the symmetry of all of the possible motions of all atom in H_2O

sum of the # of operations

number of irreducible representations of a given type needed $= \frac{1}{order} \Sigma_{classes} \left[\left(\begin{array}{c} \# \\ \text{operations} \\ \text{in class} \end{array} \right) \left(\begin{array}{c} \chi \text{ of the} \\ \text{irreducible} \\ \text{representation} \end{array} \right) \left(\begin{array}{c} \chi \text{ of the} \\ \text{reducible} \\ \text{representation} \end{array} \right) \right]$

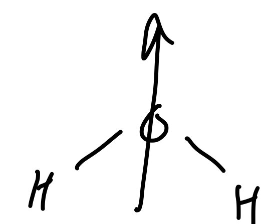
how many motions with A_1 symmetry are "hidden" in Γ

E, C_2, $\sigma_v(xz)$, $\sigma_v(yz)$

$$n(A_1) = \frac{1}{4} \cdot [(1)(1)(9) + (1)(1)(-1) + (1)(1)(3) + (1)(1)(1)]$$

$$\frac{1}{4}(9 + -1 + 3 + 1) = 3$$

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	9	-1	3	1		



There are 3 motions that have A_1 symmetry

$$\text{number of irreducible representations of a given type needed} = \frac{1}{\text{order}} \sum_{\text{classes}} \left[\left(\begin{array}{c} \# \\ \text{operations} \\ \text{in class} \end{array} \right) \left(\begin{array}{c} \chi \text{ of the} \\ \text{irreducible} \\ \text{representation} \end{array} \right) \left(\begin{array}{c} \chi \text{ of the} \\ \text{reducible} \\ \text{representation} \end{array} \right) \right]$$

$$n(A_2) = {}^1/_4 \cdot [(1)(1)(9) + (1)(1)(-1) + (1)(-1)(3) + (1)(-1)(1)]$$

$$\tfrac{1}{4}(9 + -1 + -3 + -1) = 1$$

	C_{2v}	1 E	1 C_2	$\sigma_v(xz)$	1 $\sigma_v(yz)$		
3	A_1	1	1	1	1	z	x^2, y^2, z^2
1	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	9	-1	3	1		

1 motion has A_2 symmetry

$$\text{number of irreducible representations of a given type needed} = \frac{1}{\text{order}} \sum_{\text{classes}} \left[\left(\begin{array}{c}\#\\ \text{operations}\\ \text{in class}\end{array} \right) \left(\begin{array}{c}\chi \text{ of the}\\ \text{irreducible}\\ \text{representation}\end{array} \right) \left(\begin{array}{c}\chi \text{ of the}\\ \text{reducible}\\ \text{representation}\end{array} \right) \right]$$

$\frac{1}{4}(9 + 1 + 3 + -1)$

$n(B_1) = \frac{1}{4} \cdot [(1)(1)(9) + (1)(-1)(-1) + (1)(1)(3) + (1)(-1)(1)] = 3$

	C_{2v}	1 E	1 C_2	1 $\sigma_v(xz)$	1 $\sigma_v(yz)$		
3	A_1	1	1	1	1	z	x^2, y^2, z^2
1	A_2	1	1	-1	-1	R_z	xy
3	B_1	1	-1	1	-1	x, R_y	xz
	B_2	1	-1	-1	1	y, R_x	yz
	Γ	9	-1	3	1		

number of irreducible representations of a given type needed = $^{1}/_{order}\,\Sigma_{classes}$ [(# operations in class)(χ of the irreducible representation)(χ of the reducible representation)]

$\frac{1}{4}$ (9 + 1 + -3 + 1)

$n(B_2) = {}^{1}/_{4} \cdot [(1)(1)(9) + (1)(-1)(-1) + (1)(-1)(3) + (1)(1)(1)] = 2$

	C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
3	A_1	1	1	1	1	z	x^2, y^2, z^2
1	A_2	1	1	-1	-1	R_z	xy
3	B_1	1	-1	1	-1	x, R_y	xz
2	B_2	1	-1	-1	1	y, R_x	yz
	Γ	9	-1	3	1		

2 motions have B_2 symmetry

Irreducible representations for the motions of the atoms in H_2O

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	9	-1	3	1		

2 vibrations change dipole along z

1 vibration changes dipole along x

$\Gamma = 3A_1 + A_2 + 3B_1 + 2B_2$

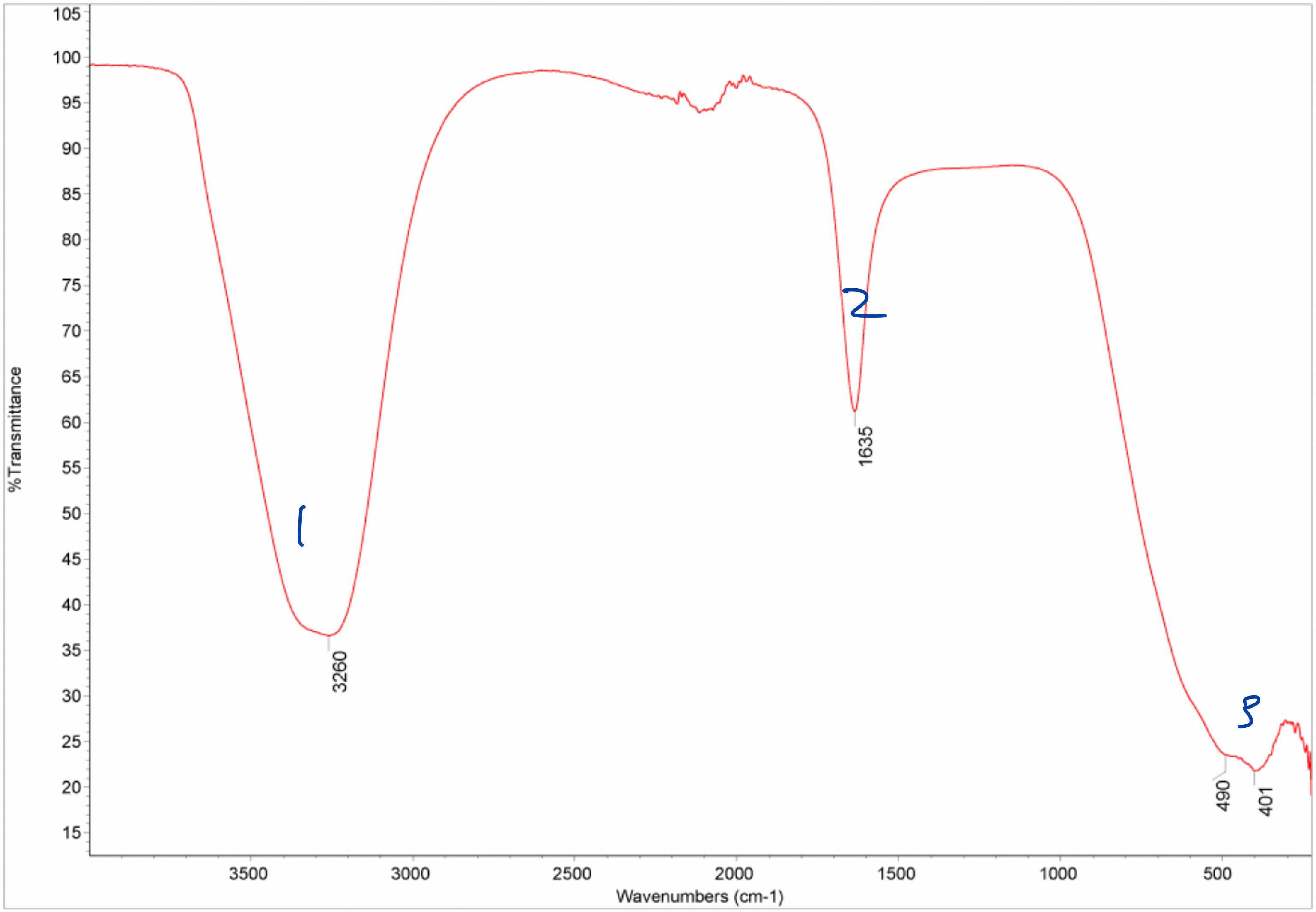
translation on x, y, & z

all possible motions = vibration + translation + rotation

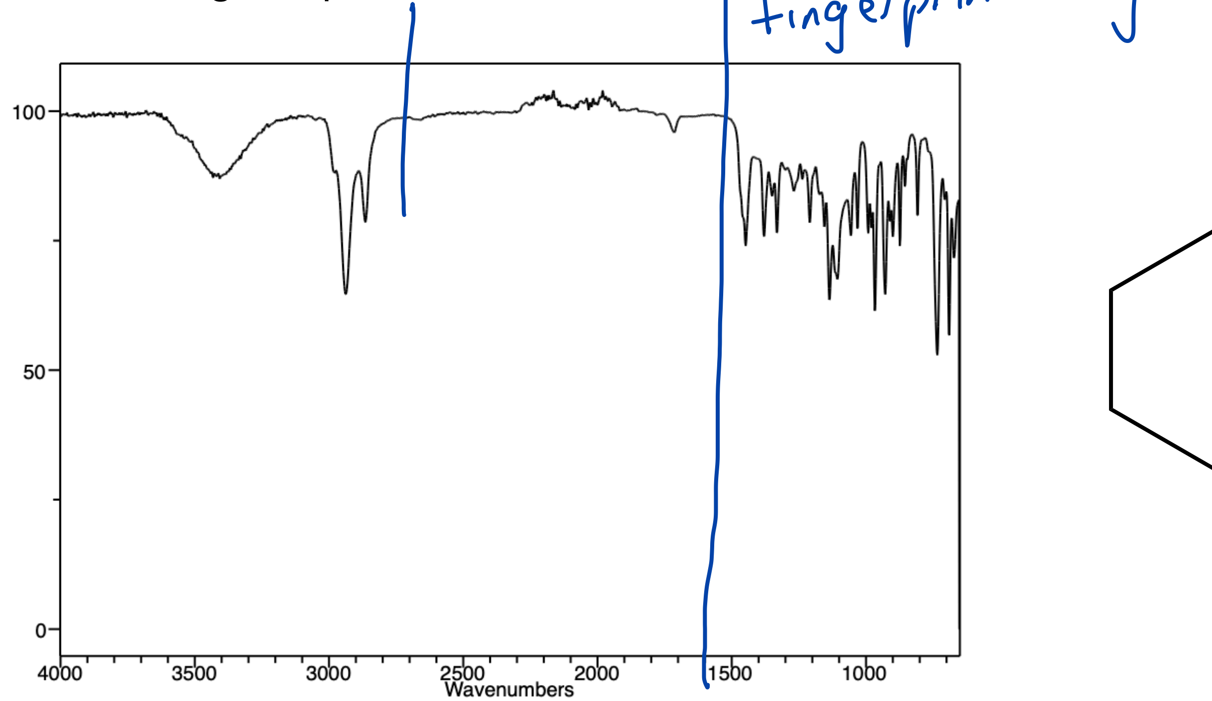
vibrational modes = $2A_1 + B_1$

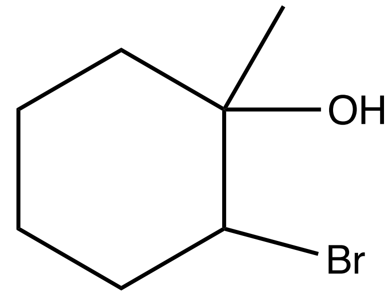
$$\text{number of vibrational modes} = \left(\text{\# of ways of moving}\right) - \left(\text{translational movement}\right) - \left(\text{rotational movement}\right)$$

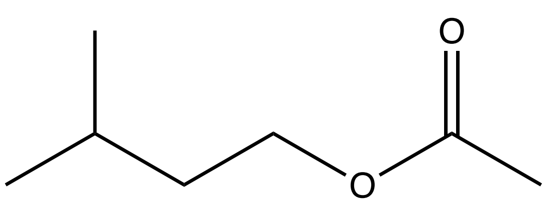
$(2\,3A_1 + A_2 + 3B_1 + 2B_2) - (A_1 + B_2 + B_1) - (A_2 + B_1 + B_2)$

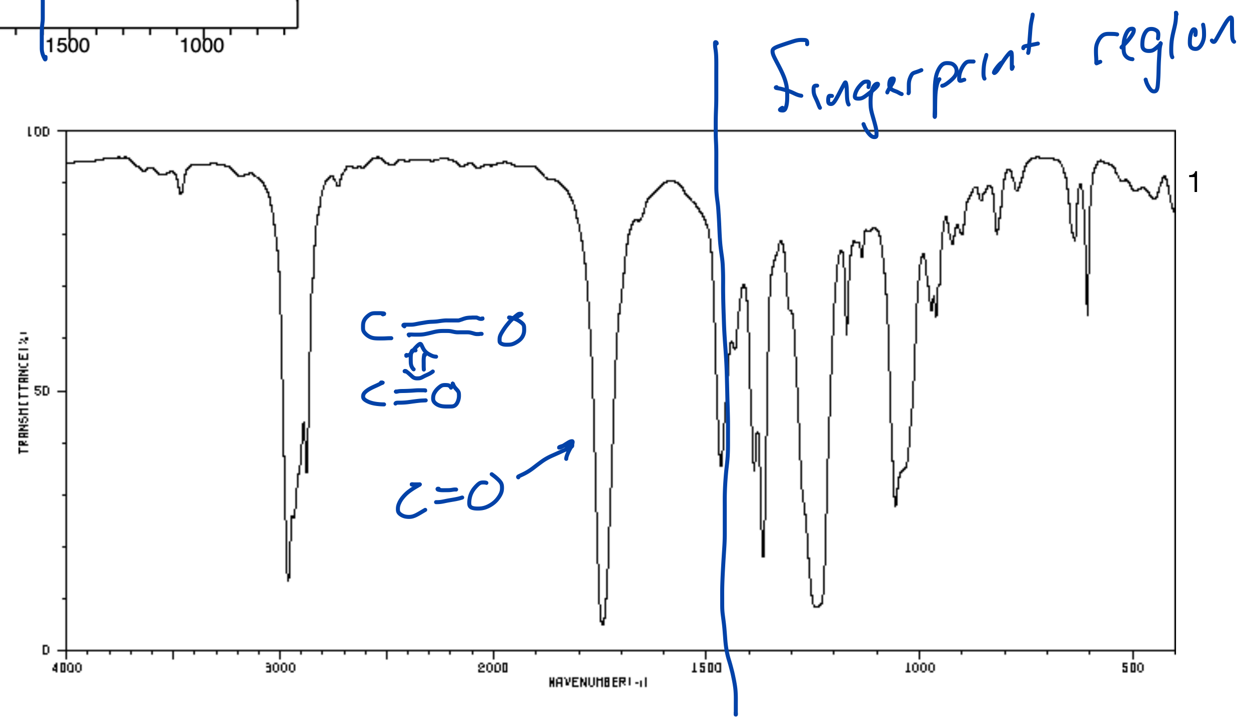


https://spectra.cs.ut.ee/conservation_materials/milli-q-water/



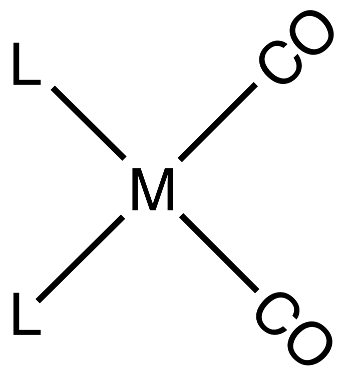


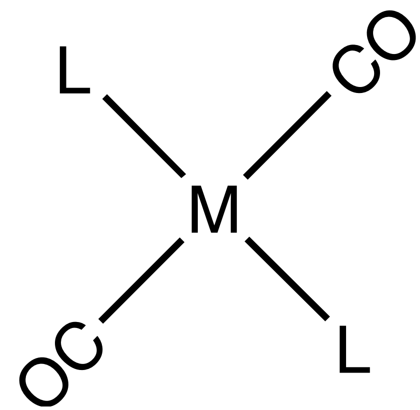


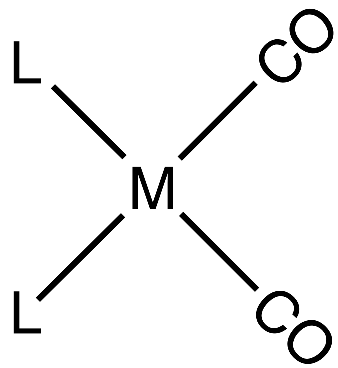


[1] https://sdbs.db.aist.go.jp/ , National Institute of Advanced Industrial Science and Technology, May 8, 2009

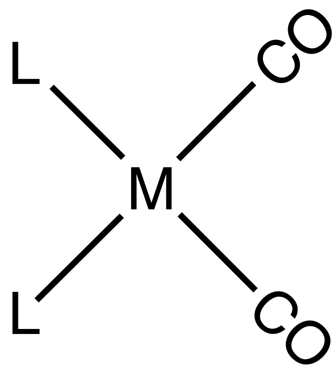
These molecules are square planar

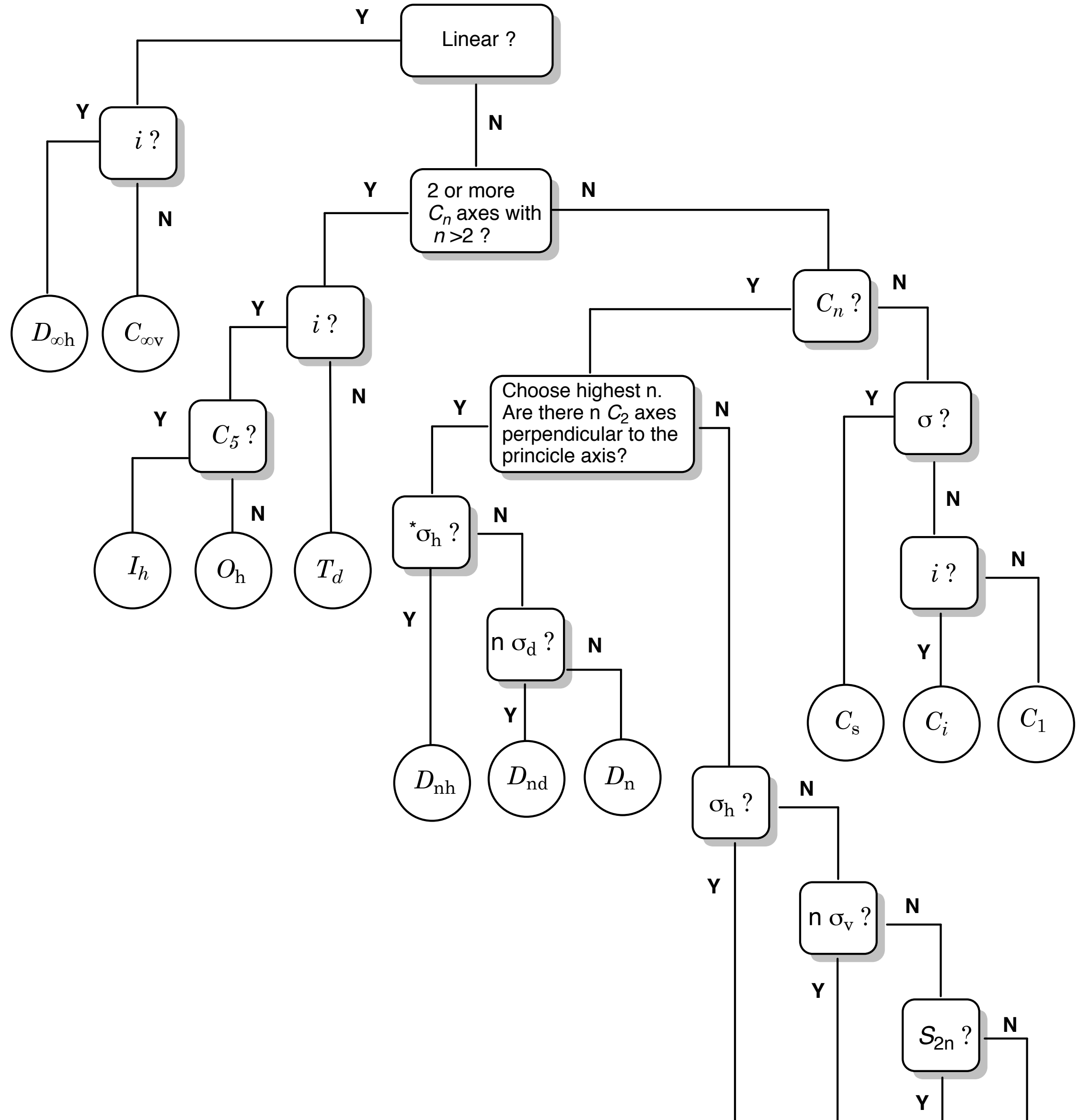





L
CO
M
L
CO

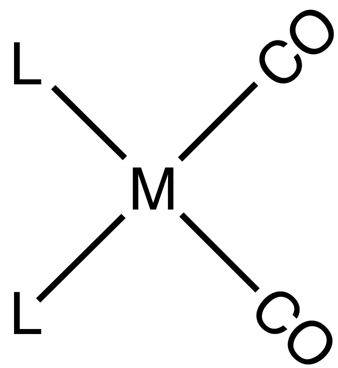
Carbonyl Stretching Bands in Metal Compounds: Find Point Group





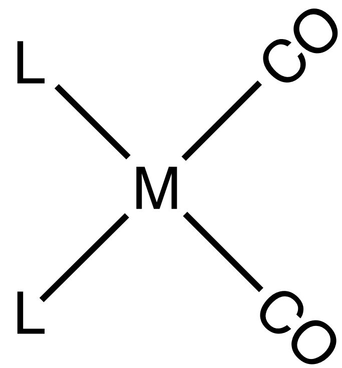
* A horizontal mirror plane is one that is perpendicular to the priciple axis. If the molecule does not posess an axis of rotation, the plane of the molecule is the horizontal mirror plane.

Carbonyl Stretching Bands in Metal Compounds: Determine Reducible Representation

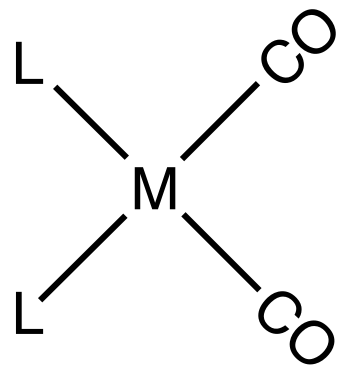


C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz
Γ						

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

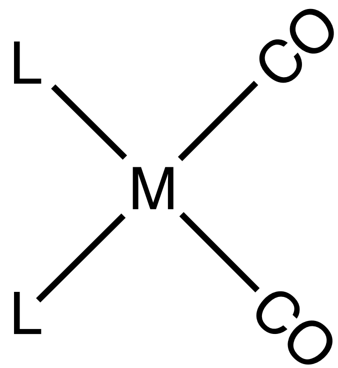


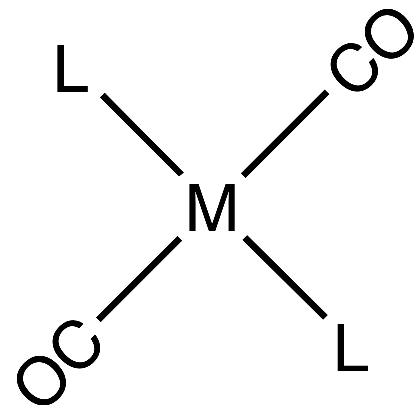
C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz
Γ	2	0	2	0		



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		

$$\Gamma = A_1 + B_1$$





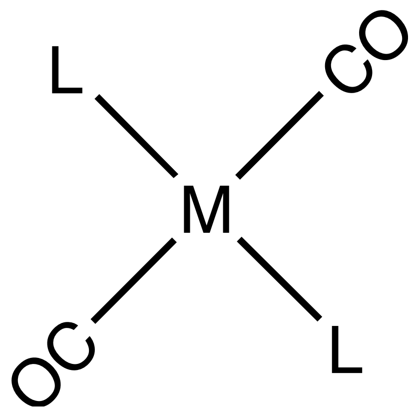
Find Rotational Axes and Assign x, y, and z Axes

Find Point Group

Determine Reducible Representation

Determine Irreducible Representations that Combine to Form Reducible Representation

Analyze Results


L
CO
M
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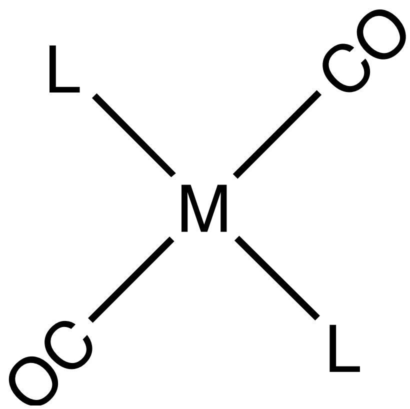
L
CO
M
OC
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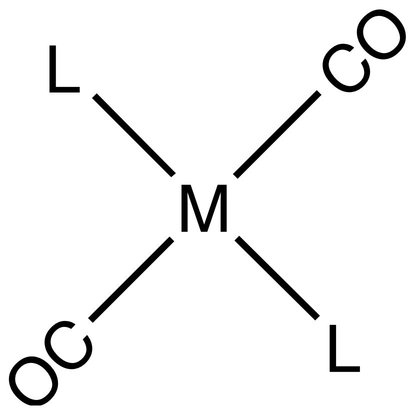
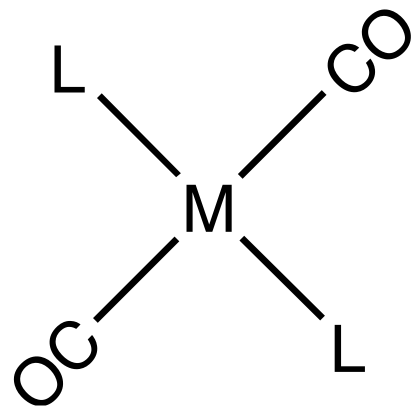
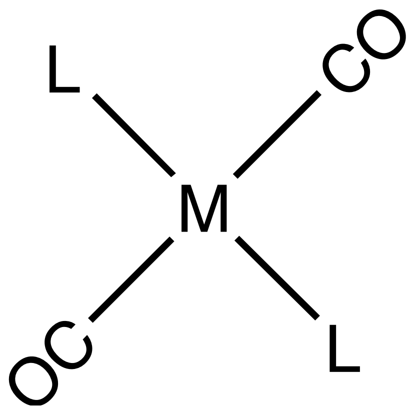


D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	*i*	$\sigma_h(xy)$	$\sigma_d(xz)$	$\sigma_d(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	xy
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y	xz
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	yz
A_u	1	1	1	1	-1	-1	-1	-1		
B_{1u}	1	1	-1	-1	-1	-1	1	1	z	
B_{2u}	1	-1	1	-1	-1	1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

Γ



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		



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		