This Class

4.3 Properties and Representations of Groups

4.4 Uses of Character Tables

Next Class

4.4 More Examples

Reworked test due on 10/20

For any question that you did not receive full credit answer that question. Please do not resubmit your actual test.

C_{2v}

identity	180° rotation	vertical mirror plane	vertical mirror plane
E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$

The set is the set of symmetry operations.
The operation is the symmetry operations operating on each other.

$C_2 \times \sigma_{v(xz)} = \sigma_{v(yz)}$ $\quad C_2 \times \sigma_{v(yz)} = \sigma_{v(xz)}$ $\quad \sigma_{v(xz)} \times \sigma_{v(yz)} = C_2$

$C_2 \times (\sigma_{v(xz)} \times C_2) = \sigma_{v(xz)}$ $\quad (C_2 \times \sigma_{v(xz)}) \times C_2 = \sigma_{v(xz)}$

$E \times C_2 = C_2$

$C_2 \times C_2 = E$

letters, drawings,

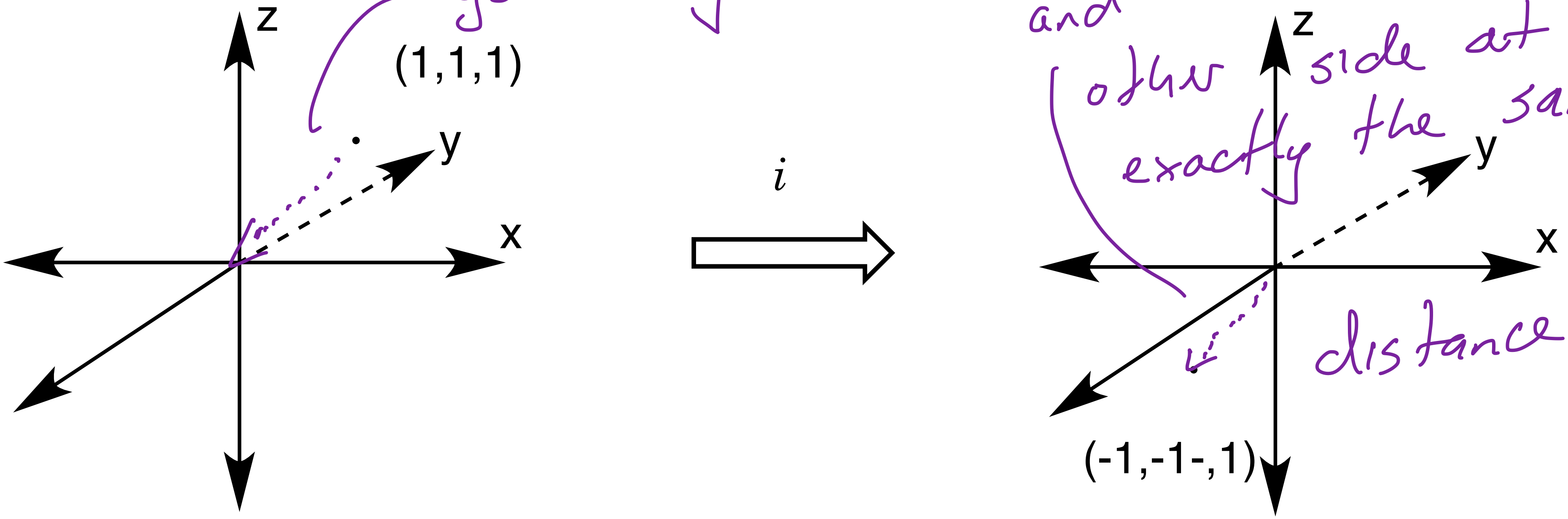
E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$	
$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	
what happen on				
1	-1	1	-1	x
1	-1	-1	1	y
1	1	1	1	z
3	-1	1	1	

transformation matrices

trace of the transformation matrix

sum the characters along the diagonal

Transformation Matrices



go through center and come out the other side at exactly the same distance

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} \qquad \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \qquad \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

original coord

transformation matrix

new coord

Matrix Multiplication…

Number of columns in the first matrix must equal number of rows in the second

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

new x value = sum of Row 1 x Column 1

new y value = sum of Row 2 x Column 1

new z value = sum of Row 3 x Column 1

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -1(x) + 0(y) + 0(z) \\ 0(x) + -1(y) + 0(z) \\ 0(x) + 0(y) + -1(z) \end{bmatrix}$$

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -x \\ -y \\ -z \end{bmatrix}$$

Summary of all symmetry of the point group

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

order is the # of symmetry operations

irreducible representations = # of classes

*Δ Mulliken Labels σ + π related to symmetry in simple diatomic molecules

these are the characters

the colums are the "classes" there are 4 classes in the C_{2v} point group. A class contains symmetry operations that give the same characters

Anything that is related to symmetry

motions of a molecule

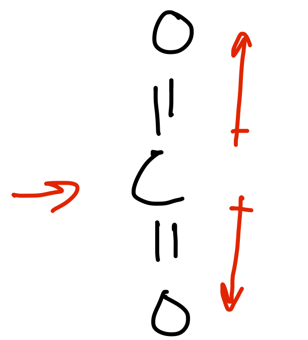
vibrational spectroscopy IR + Raman

interaction of orbitals to form molecular orbitals

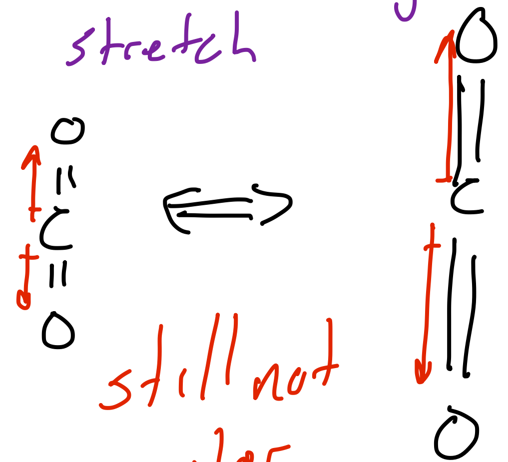
vibrational modes

this is a symmetrical stretch

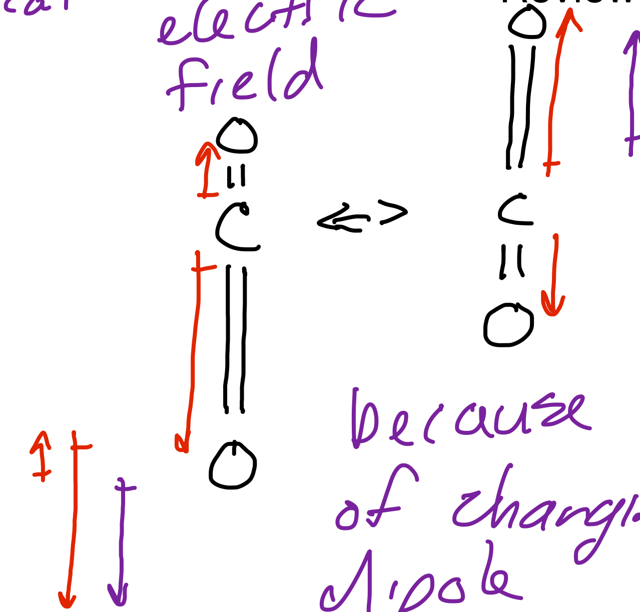
oscillating electric field



not polar



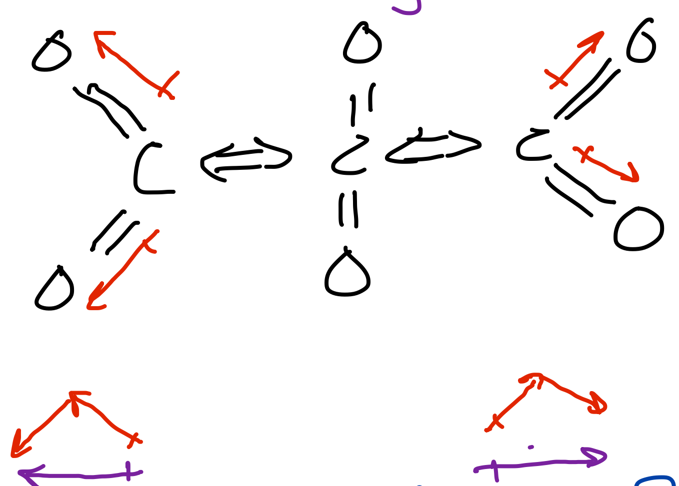
still not polar

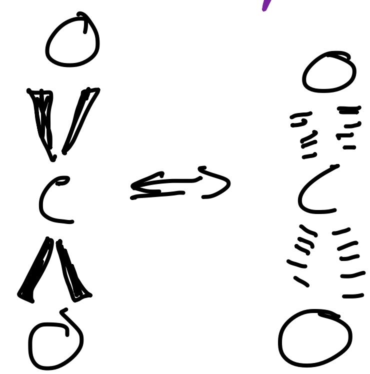


because of changing dipole

bending

vibrations that change the dipole are IR active





bending

When a vibration changes the dipole of the molecule an oscillating electric field is created... which interacts with other oscillating electric fields. IR photons

Use character tables to determine the symmetry of the molecule's vibrations to determine how many IR bands (peaks) will be present. today

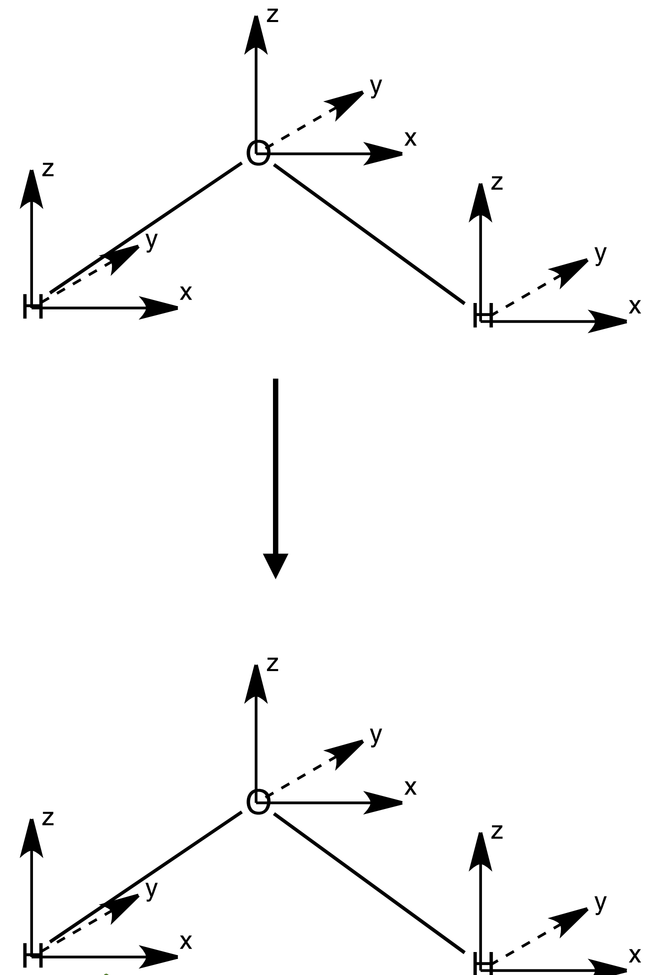
We can also use character tables to examine specific kinds of vibrations. next class

Number of IR Active Vibrational Modes for Water

reducible representation

C_{2v}	**E**	C_2	$\sigma_{(xz)}$	$\sigma_{(yz)}$
Γ	9			

$$
\begin{array}{ll}
O & x'_O \\
 & y'_O \\
 & z'_O \\
H_a & x'_{Ha} \\
 & y'_{Ha} \\
 & z'_{Ha} \\
H_b & x'_{Hb} \\
 & y'_{Hb} \\
 & z'_{Hb}
\end{array}
=
\begin{array}{|c|c|c|c|c|c|c|c|c|}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
 & & & 1 & & & & & \\
 & & & & 1 & & & & \\
 & & & & & 1 & & & \\
 & & & & & & 1 & & \\
 & & & & & & & 1 & \\
 & & & & & & & & 1
\end{array}
\begin{array}{l}
x_O \\ y_O \\ z_O \\ x_{Ha} \\ y_{Ha} \\ z_{Ha} \\ x_{Hb} \\ y_{Hb} \\ z_{Hb}
\end{array}
$$

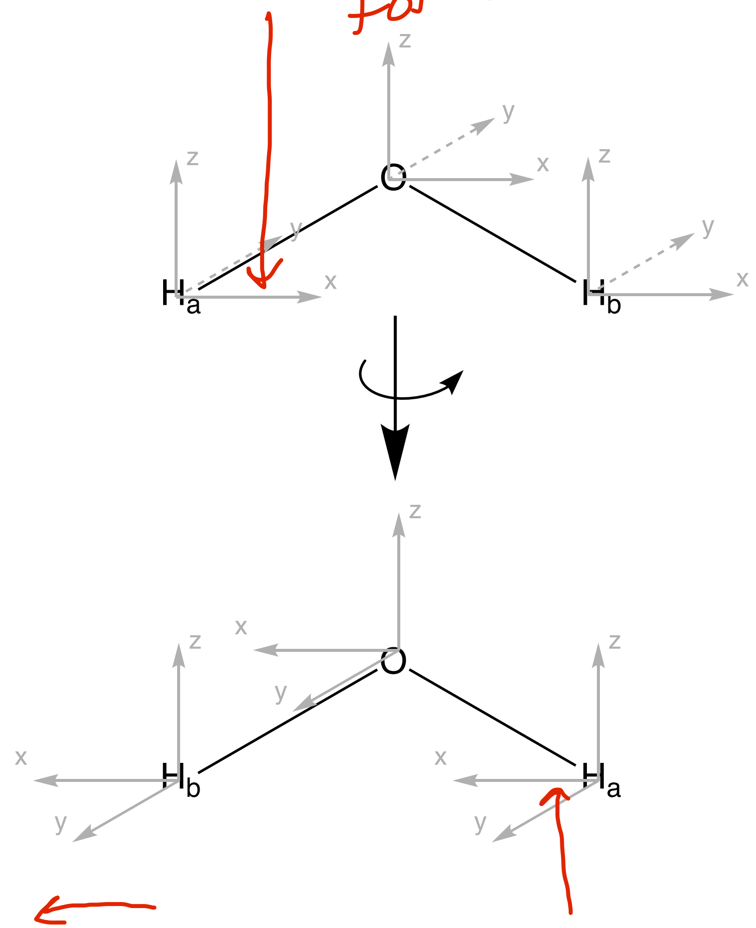


the trace of the transformation matrix is a summary of the information about what happens to the movement of the atoms when we do the E operation

C_{2v}	E	C_2	$\sigma_{(xz)}$	$\sigma_{(yz)}$
	9	-1		

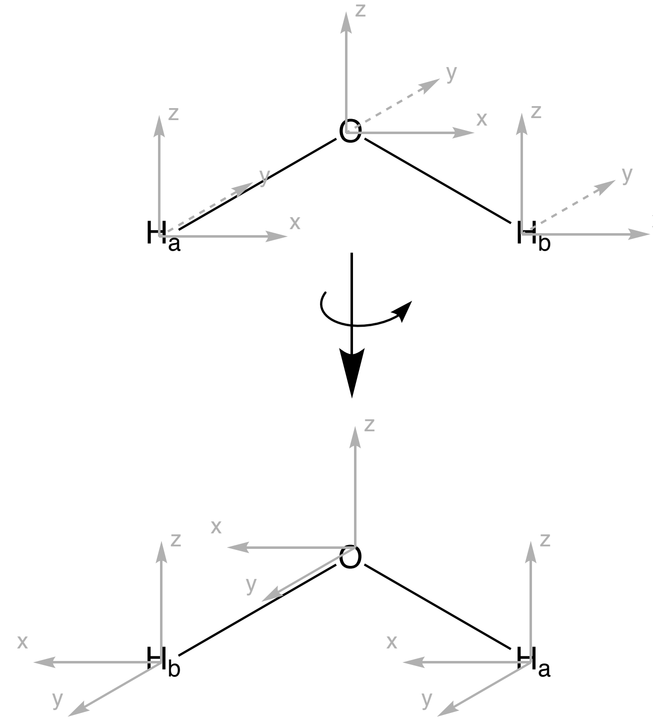
$$\begin{array}{cc} \mathrm{O} & x'_O \\ & y'_O \\ & z'_O \\ \mathrm{H_a} & x'_{Ha} \\ & y'_{Ha} \\ & z'_{Ha} \\ \mathrm{H_b} & x'_{Hb} \\ & y'_{Hb} \\ & z'_{Hb} \end{array} = \begin{array}{|ccccccccc|} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{array} \begin{array}{c} x_O \\ y_O \\ z_O \\ x_{Ha} \\ y_{Ha} \\ z_{Ha} \\ x_{Hb} \\ y_{Hb} \\ z_{Hb} \end{array}$$

original x vector for Ha



C_{2v}	E	$\mathbf{C_2}$	$\sigma_{(xz)}$	$\sigma_{(yz)}$
	9	-1		

$$\begin{array}{ll} \mathrm{O} & x'_{O} \\ & y'_{O} \\ & z'_{O} \\ \mathrm{H_a} & x'_{Ha} \\ & y'_{Ha} \\ & z'_{Ha} \\ \mathrm{H_b} & x'_{Hb} \\ & y'_{Hb} \\ & z'_{Hb} \end{array} = \begin{bmatrix} -1 & & & & & & & & \\ & -1 & & & & & & & \\ & & 1 & & & & & & \\ & & & 0 & & & -1 & & \\ & & & & 0 & & & -1 & \\ & & & & & 0 & & & 1 \\ & & & -1 & & & 0 & & \\ & & & & -1 & & & 0 & \\ & & & & & 1 & & & 0 \end{bmatrix} \begin{array}{l} x_{O} \\ y_{O} \\ z_{O} \\ x_{Ha} \\ y_{Ha} \\ z_{Ha} \\ x_{Hb} \\ y_{Hb} \\ z_{Hb} \end{array}$$



easier way to do this? Yes.

dont change position don't change sign 1

dont change position but sign changes -1

change the position contributes 0 to the trace