(11) **Today**

4.3 Character Tables

4.4 Uses of Character Tables

Next Class (12)

4.4 Uses of Character Tables

Second Class from Today

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

Third Class from Today (13)

4.4 Uses of Character Tables

operations

functions

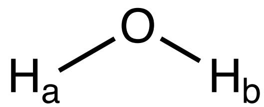
C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

labels

characters

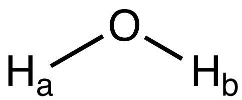
classes

a summary of all of the symmetry in a given point group

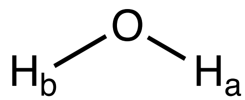


C_{2v} operations: E, C_2, $\sigma_v(xz)$, $\sigma_v(yz)$

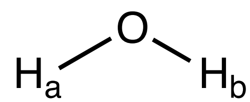
E



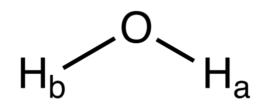
C_2



$\sigma_v(xz)$



$\sigma_v(yz)$



Matrix representations

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

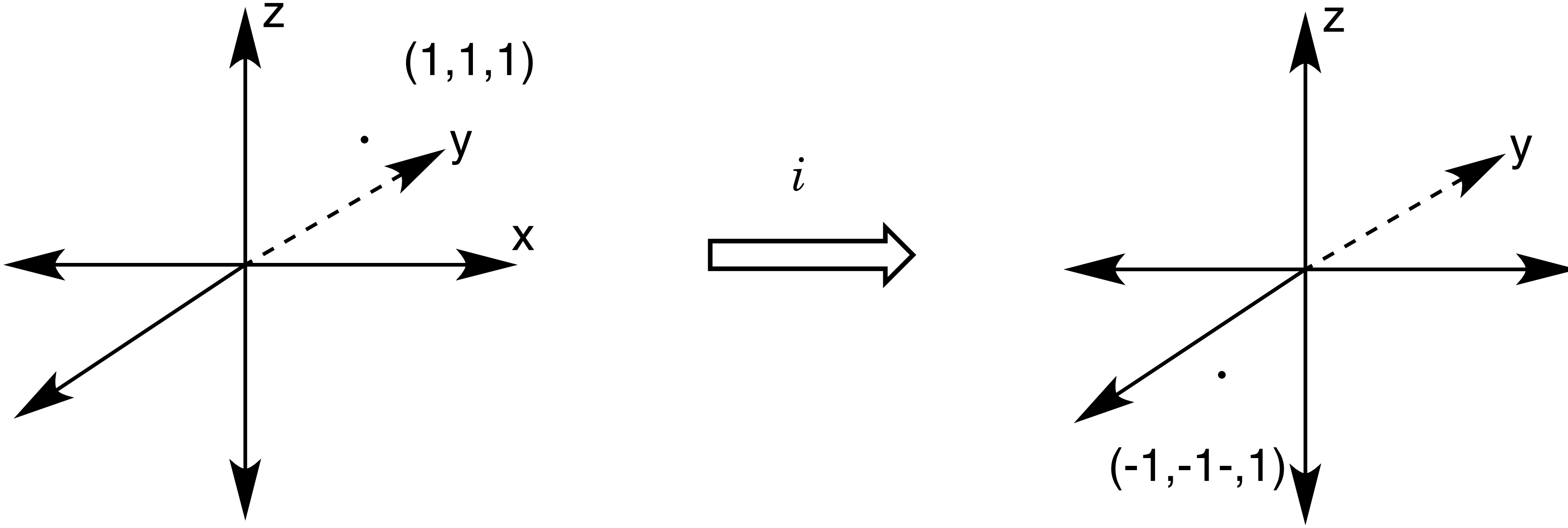
1x1 transformation matrices for each individual axis

1	-1	1	-1	x
1	-1	-1	1	y
1	1	1	1	z

The traces of the 3x3 transformation matices

3	-1	1	1

Transformation Matrices



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

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

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

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

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

1x1 transformation matrices for each individual axis in the C_{2v} point group

1	-1	1	-1	x
1	-1	-1	1	y
1	1	1	1	z

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

Muliken symbols summary symmetry for each irreducible representation

symmetric

antisymmetric – thing doesn't move but its sign changes (phase of p orbital dir

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

A Symmetric w.r.t. principle axis
B antisymmetric w.r.t. principle axis
subscript 1 is for representations that are symmetric w.r.t. a C_2 that is perpendicular to the principle axis
subscript 2 is for representations that are antisymmetric w.r.t. a C_2 that is perpendicular to the principle axis
in the absence of a C_2 a vertical mirror plane perpendicular to the plane of the molecule is used instead
subscript g symmetric w.r.t. inversion
subscript u antisymmetric w.r.t. inversion
' symmetric w.r.t. σ_h
'' antisymmetric w.r.t. σ_h

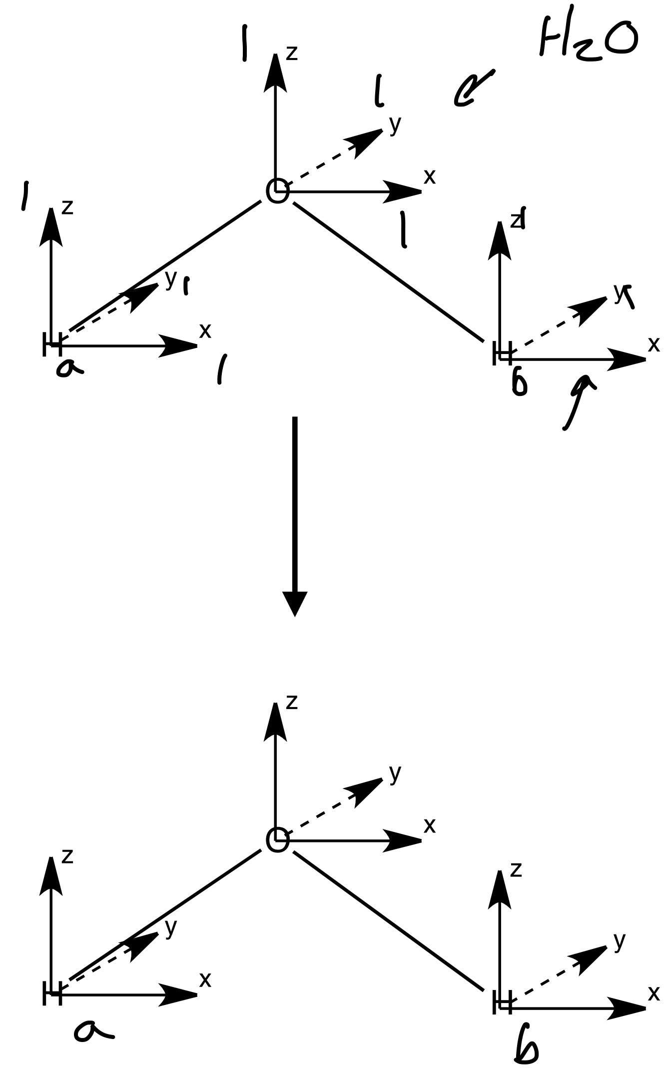
How do we use Character Tables.

To examine the symmetry of the thing we are interested in (molecular motions, orbitals, symmetry adapted linear combinations of atomic orbitals...) we create a reducible representation of the symmetry operations of the motions.		For each operation and each item add 1, 0 or -1 to the value for χ based on whether there is no change (1), the items changes position (0), or doesn't change position but changes sign (-1).
We use linear algebra to determine the irreducible representations that must be combined to form the reducible one that we just found.		
We use the functions in the character tables to interpret our results.		

Find this by analyzing all possible motions of the atoms in H_2O

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

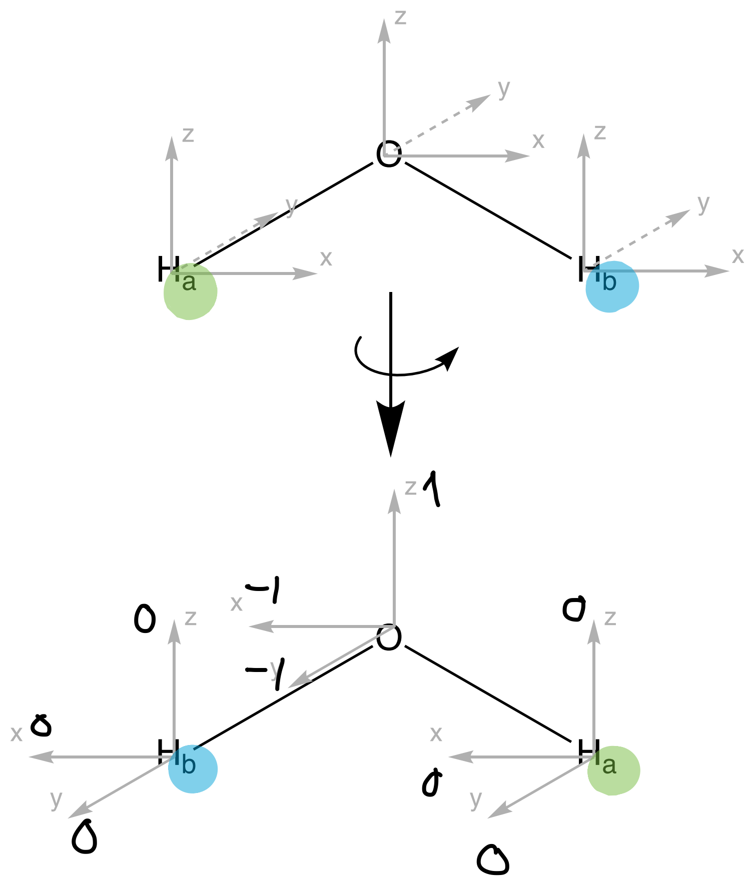
$$
\begin{matrix} O \\ \\ \\ H_a \\ \\ \\ H_b \\ \\ \\ \end{matrix}
\begin{pmatrix} x'_O \\ y'_O \\ z'_O \\ x'_{Ha} \\ y'_{Ha} \\ z'_{Ha} \\ x'_{Hb} \\ y'_{Hb} \\ z'_{Hb} \end{pmatrix}
=
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix} x_O \\ y_O \\ z_O \\ x_{Ha} \\ y_{Ha} \\ z_{Ha} \\ x_{Hb} \\ y_{Hb} \\ z_{Hb} \end{pmatrix}
$$



summarize this matrix using its trace 9 which is the sum of the diagonal

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

O	x'_O	-1	0	0	0	0	0	0	0	0	x_O
	y'_O	0	-1	0	0	0	0	0	0	0	y_O
	z'_O	0	0	1	0	0	0	0	0	0	z_O
H_a	x'_{Ha}	0	0	0	0	0	0	-1	0	0	x_{Ha}
	y'_{Ha} =	0	0	0	0	0	0	0	-1	0	y_{Ha}
	z'_{Ha}	0	0	0	0	0	0	0	0	1	z_{Ha}
H_b	x'_{Hb}	0	0	0	-1	0	0	0	0	0	x_{Hb}
	y'_{Hb}	0	0	0	0	-1	0	0	0	0	y_{Hb}
	z'_{Hb}	0	0	0	0	0	1	0	0	0	z_{Hb}



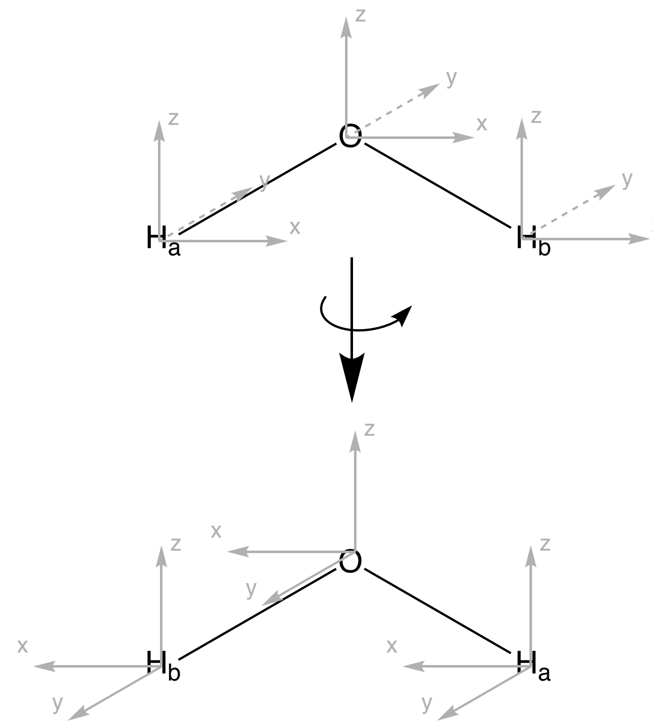
trace = -1

create the characters for the reducible representation for all the possible motions

did it change position no
did it change sign or direction
add 1 for each vector that did nothing

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

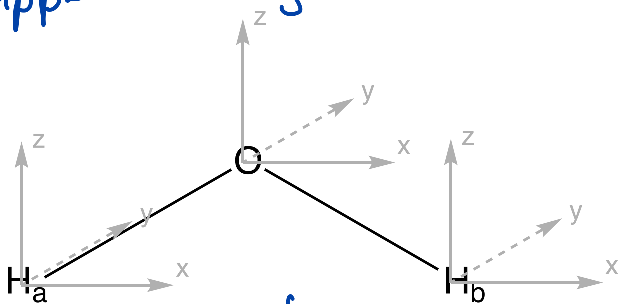
O	x'_O		-1									x_O
	y'_O			-1								y_O
	z'_O				1							z_O
H_a	x'_{Ha}					0			-1			x_{Ha}
	y'_{Ha}	=					0			-1		y_{Ha}
	z'_{Ha}							0			1	z_{Ha}
H_b	x'_{Hb}					-1			0			x_{Hb}
	y'_{Hb}						-1			0		y_{Hb}
	z'_{Hb}							1			0	z_{Hb}

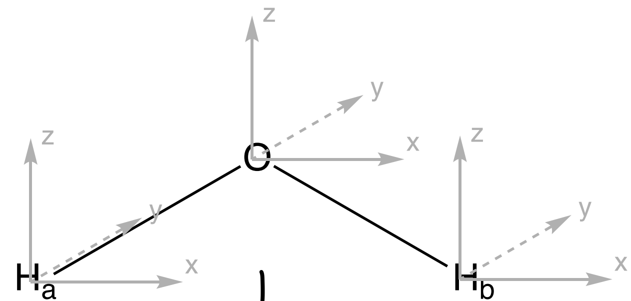


For each operation add 1, 0 or -1 to the value for χ based on whether there is no change (1), the items changes position (0), or doesn't change position but changes sign (-1).

C_{2v}	E	C_2	$\sigma_{(xz)}$	$\sigma_{(yz)}$
Γ	9	-1	3	1

upper case gamma





$\sigma_{(xz)}$

$\sigma_{(yz)}$

For each operation add 1, 0 or -1 to the value for χ based on whether there is no change (1), the items changes position (0), or doesn't change position but changes sign (-1).