Every molecule has a point group associated with it, which are assigned by a set for rules (explained by Group theory). The character tables takes the point group and represents all of the symmetry that the molecule has.

Symbols under the first column of the character tables

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A (Mulliken Symbol)</td>
<td>(singly degenerate or one dimensional) symmetric with respect to rotation of the principle axis</td>
</tr>
<tr>
<td>B (Mulliken Symbol)</td>
<td>(singly degenerate or one dimensional) anti-symmetric with respect to rotation of the principle axis</td>
</tr>
<tr>
<td>E (Mulliken Symbol)</td>
<td>(doubly degenerate or two dimensional)</td>
</tr>
<tr>
<td>T (Mulliken Symbol)</td>
<td>(thirdly degenerate or three dimensional)</td>
</tr>
</tbody>
</table>

Subscript 1

- symmetric with respect to the C\(_n\) principle axis, if no perpendicular axis, then it is with respect to \(\sigma_v\)

Subscript 2

- anti-symmetric with respect to the C\(_n\) principle axis, if no perpendicular axis, then it is with respect to \(\sigma_v\)

Subscript g

- symmetric with respect to the inverse

Subscript u

- anti-symmetric with respect to the inverse

Prime

- symmetric with respect to \(\sigma_h\) (reflection in horizontal plane)

Double prime

- anti-symmetric with respect to \(\sigma_h\) (opposite reflection in horizontal plane)

Symbols in the first row of the character tables

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>describes the degeneracy of the row (A and B= 1) (E=2) (T=3)</td>
</tr>
<tr>
<td>C(_n)</td>
<td>(2\pi/n) = number of turns in one circle on the main axis without changing the look of a molecule (rotation of the molecule)</td>
</tr>
<tr>
<td>C(_n)'</td>
<td>(2\pi/n) = number of turns in one circle perpendicular to the main axis, without changing the structure of the molecule</td>
</tr>
<tr>
<td>C(_n)&quot;</td>
<td>(2\pi/n) = number of turns in one circle perpendicular to the (C_n') and the main axis, without changing the structure</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>(\sigma')</td>
<td>reflection of the molecule perpendicular to the other sigma</td>
</tr>
<tr>
<td>(\sigma_v) (vertical)</td>
<td>reflection of the molecule vertically compared to the horizontal highest fold axis.</td>
</tr>
<tr>
<td>(\sigma_h) or (\sigma_d) (horizontal)</td>
<td>reflection of the molecule horizontally compared to the horizontal highest fold axis.</td>
</tr>
<tr>
<td>(i)</td>
<td>Inversion of the molecule from the center</td>
</tr>
<tr>
<td>(S_n)</td>
<td>rotation of (2\pi/n) and then reflected in a plane perpendicular to rotation axis.</td>
</tr>
<tr>
<td>(#C_n)</td>
<td>the # stands for the number of irreducible representation for the (C_n)</td>
</tr>
<tr>
<td>(#\sigma)</td>
<td>the # stands for the number irreducible representations for the sigmas.</td>
</tr>
<tr>
<td></td>
<td>in the same rotation there is another rotation, for instance (O_h) has (3C_2=C_4^2)</td>
</tr>
<tr>
<td></td>
<td>other useful definitions</td>
</tr>
<tr>
<td>((R_x,R_y))</td>
<td>the ((,) means they are the same and can be counted once.</td>
</tr>
<tr>
<td>(x^2+y^2, z^2)</td>
<td>without ((,) means they are different and can be counted twice.</td>
</tr>
</tbody>
</table>

**Looking at a Character Table**

<table>
<thead>
<tr>
<th>(D_{3h})</th>
<th>E</th>
<th>(2C_3)</th>
<th>(3C_2)</th>
<th>(\sigma_h)</th>
<th>(2S_3)</th>
<th>(3\sigma_v)</th>
<th>IR</th>
<th>Raman</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A_1')</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>(x^2+y^2, z^2)</td>
<td></td>
</tr>
<tr>
<td>(A_2')</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>(R_z)</td>
<td></td>
</tr>
<tr>
<td>(E')</td>
<td>2</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>-1</td>
<td>0</td>
<td>((x,y))</td>
<td>((x^2-y^2, xy))</td>
</tr>
<tr>
<td>(A_1'')</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(A_2'')</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>(z)</td>
<td></td>
</tr>
</tbody>
</table>
The order is the number in front of the the classes. If there is not number then it is considered to be one. The number of classes is the representation of symmetries. The D₃h has six classes and an order of twelve.

### Understanding using matrix

The identity does nothing to the matrix.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} X \\ Y \\ Z \end{bmatrix}$$

$$\sigma(xy)$$ the x and y stay positive, while z turns into a negative.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} X \\ Y \\ -Z \end{bmatrix}$$

Inversion (I) is when all of the matrix turns into a negative.

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} -X \\ -Y \\ -Z \end{bmatrix}$$

$$C_n$$is when one would use cos and sin. For an example C₄

$$\begin{bmatrix} \cos \left( \frac{2\pi}{4} \right) \hspace{0.5cm} -\sin \left( \frac{2\pi}{4} \right) \\ \sin \left( \frac{2\pi}{4} \right) \hspace{0.5cm} \cos \left( \frac{2\pi}{4} \right) \\ 0 \hspace{0.5cm} 0 \hspace{0.5cm} 1 \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} \end{bmatrix}$$

### References

Practice

There are two columns on the far right. One is IR and the other is Raman. Try moving the molecule around using reflections and rotations. Remember when the positive side of the orbitals goes into the negative side, the number is negative (in the character tables). Also, remember if it is moved or reflected and there is no change then the number is positive (in the character tables). Also, molecules are placed on a x, y, and z (three dimensional) graph. The highest C fold rotation is always on the z axis.

<table>
<thead>
<tr>
<th>IR</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(P_x)</td>
<td></td>
</tr>
<tr>
<td>(P_y)</td>
<td></td>
</tr>
<tr>
<td>(P_z)</td>
<td></td>
</tr>
<tr>
<td>(R_x)</td>
<td></td>
</tr>
<tr>
<td>(R_y)</td>
<td></td>
</tr>
<tr>
<td>(R_z)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Raman</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(\sigma)</td>
<td></td>
</tr>
<tr>
<td>(d_{xy})</td>
<td></td>
</tr>
<tr>
<td>(d_{yz})</td>
<td></td>
</tr>
<tr>
<td>(d_{xz})</td>
<td></td>
</tr>
<tr>
<td>(d_{z^2})</td>
<td></td>
</tr>
<tr>
<td>(d_{x^2-y^2})</td>
<td></td>
</tr>
</tbody>
</table>