Symmetry Operation: a movement of an object such that, after the movement has been carried out, every point on the object is coincident with an equivalent point (or the same point) of the object in its original orientation.

Symmetry Element: geometrical entity; a point, line or plane; with respect to which one or more symmetry operations may be carried out.

Group Theory

All symmetry elements in molecule, collected together, form a: mathematical group

1. **product** of 2 group elements = a group element: \( AB = C \)
   
   *B followed* by A same as C

2. has **identity** operator: \( EA = A \)

3. each element has **inverse**; also a group element: \( A^{-1}A = E \)
Point Groups

Point groups represented (shorthand) by:

Schoenflies symbol

\[
\begin{align*}
C_1 & \quad E \\
C_i & \quad E, i \\
C_2 & \quad E, \sigma \\
C_2' & \quad E, C_2 \\
D_3 & \quad E, 2 C_3, 3 C_2 \\
C_{2h} & \quad E, C_2, \sigma_v(xy), \sigma_v(yz) \\
C_{3h} & \quad E, 2 C_3, 3 \sigma_v \\
C_{3v} & \quad E, i, C_2, \sigma_h \\
C_{3h} & \quad E, C_3, \sigma_h, S_3 \\
D_{2h} & \quad E, 2 S_d, C_2, 2 C_2', 2 \sigma_d \\
D_{3d} & \quad E, 2 C_3, 3 C_2, i, 2 S_d, 3 \sigma_d \\
D_{2d} & \quad E, C_2(x), C_2(y), C_2(z), i, \sigma_v(xy), \sigma_v(xz), \sigma_v(yz) \\
D_{3h} & \quad E, 2 C_3, 3 C_2, \sigma_h, 2 S_d, 3 \sigma_v \\
D_{3d} & \quad E, 8 C_3, 3 C_2, 6 S_d, 6 \sigma_d \\
O_h & \quad E, 8 C_3, 6 C_2, 6 C_4, 3 C_2, i, 6 S_4, 8 S_6, 3 \sigma_d, 6 \sigma_d \\
C_{4h} & \quad E, 2 C_{4v}, \infty \sigma_v \\
D_{4h} & \quad E, 2 C_{4v}, \infty \sigma_v, i, 2 S_{4v}, \infty C_2 \\
I_h & \quad E, 12 C_3, 20 C_3, 15 C_2, i, 12 S_{10}, 20 S_{10}, 15 \sigma
\end{align*}
\]

all elements not needed to assign point group:

Arthur Schönflies
German
1891

Flowchart for Identifying Molecular Point Groups
Flowchart for Identifying Molecular Point Groups

Flowchart for Identifying Molecular Point Groups
Flowchart for Identifying Molecular Point Groups...

[Images of molecular structures and flowchart diagrams related to identifying molecular point groups.]
Flowchart for Identifying Molecular Point Groups

Examples
Examples

\[ \text{Examples} \]

[Chemical structures of various compounds are shown, including benzene rings, metal complexes, and organic molecules.]

[Diagram showing chemical structures including benzene rings, metal complexes, and organic molecules.]
Examples

\begin{align*}
\text{Examples} & \\
\text{Examples} & \\
\end{align*}
Examples

$C_4$

$\text{Examples}$

$\sigma$

$\sigma$

$\text{Examples}$
Examples

Rhinovirus

Examples

sphere:
### Character Table

<table>
<thead>
<tr>
<th>$C_{2v}$</th>
<th>$E$</th>
<th>$C_2$</th>
<th>$\sigma_v(xz)$</th>
<th>$\sigma_v'(yz)$</th>
<th>$z$</th>
<th>$x^2, y^2, z^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$z$</td>
<td></td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>$R_z$</td>
<td>$xy$</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>$x, R_y$</td>
<td>$xz$</td>
</tr>
<tr>
<td>$B_2$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>$y, R_x$</td>
<td>$yz$</td>
</tr>
</tbody>
</table>

$A, B$ character under $C_n$ is $+,-$

$1, 2$ character under $\sigma_v$ or $C_2 \perp$ to $C_n$ is $+,-$

$', ''$ character under $\sigma_h$ is $+,-$

$g, u$ character under $t$ is $+,-$ (gerade, ungerade)

$E$ character under $E$ is $2$, (2-dimensional)

$T$ character under $E$ is $3$, (3-dimensional)

### $O_h$ Character Table

<table>
<thead>
<tr>
<th>$O_h$</th>
<th>$E$</th>
<th>$8C_3$</th>
<th>$6C_2$</th>
<th>$6C_4$</th>
<th>$3C_2$</th>
<th>$i$</th>
<th>$6S_1$</th>
<th>$8S_2$</th>
<th>$3\sigma_0$</th>
<th>$6\sigma_d$</th>
<th>$x^2+y^2+z^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{1g}$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>$R_x, R_y, R_z$</td>
</tr>
<tr>
<td>$A_{2g}$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>$x, y, z$</td>
</tr>
<tr>
<td>$E_g$</td>
<td>2</td>
<td>-1</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>-1</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>$(x^2, x^2-y^2)$</td>
</tr>
<tr>
<td>$T_{1g}$</td>
<td>3</td>
<td>0</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>3</td>
<td>1</td>
<td>0</td>
<td>-1</td>
<td>-1</td>
<td>$(xz, yz, xy)$</td>
</tr>
<tr>
<td>$T_{2g}$</td>
<td>3</td>
<td>0</td>
<td>-1</td>
<td>-1</td>
<td>3</td>
<td>-1</td>
<td>0</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$A_{1u}$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$A_{2u}$</td>
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<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$E_u$</td>
<td>2</td>
<td>-1</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>-2</td>
<td>0</td>
<td>1</td>
<td>-2</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$T_{1u}$</td>
<td>3</td>
<td>0</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>-3</td>
<td>-1</td>
<td>-1</td>
<td>0</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$T_{2u}$</td>
<td>3</td>
<td>0</td>
<td>1</td>
<td>-1</td>
<td>-3</td>
<td>1</td>
<td>0</td>
<td>-1</td>
<td>0</td>
<td>-1</td>
<td></td>
</tr>
</tbody>
</table>
Reducing Reducible Representations

\[ N = \frac{1}{h} \sum_x \chi_r^x \chi_i^x n^x \]

- \( N \) \# of times irreducible representation occurs
- \( \chi_r^x, \chi_i^x \) characters of reducible representation and irreducible representation under class \( x \)
- \( h \) order = total of symmetry operations
- \( n^x \) \# of operations in class

Optical Activity
Symmetry and NMR

Bonding and Orbitals

Orbitals have same symmetry as character table functions.

\[
\begin{align*}
D_{sh} & | E & 2C_3^1 & 3C_2^1 & i & 2S_0 & 3\sigma_v \\
A_1 & 1 & 1 & 1 & 1 & 1 & 1 \\
A_2 & 1 & 1 & -1 & 1 & 1 & -1 \\
E & 2 & -1 & 0 & 0 & 0 & 0 \\
A_{1u} & 1 & 1 & 1 & -1 & -1 & 1 \\
A_{2u} & 1 & 1 & -1 & -1 & 1 & z \\
E_{u} & 2 & -1 & 0 & -2 & 1 & 0 \\
R & x^2 + y^2, z^2 & R_e & (x^2 - y^2, xy), (xz, yz) \\
R_p & (x, y) & & \end{align*}
\]
Bonding and Orbitals

orbitals have same symmetry as character table functions

\[
\begin{array}{c|c c c c|c}
D_{ad} & E & 2C_{s} & 3C_{2} & i & 2S_{a} \ 3\sigma_{g} \\
\hline
A_{1g} & 1 & 1 & 1 & 1 & 1 \\
A_{2g} & 1 & 1 & -1 & 1 & 1 \\
E_{g} & 2 & -1 & 0 & 2 & -1 \\
A_{1u} & 1 & 1 & 1 & -1 & -1 \\
A_{2u} & 1 & 1 & -1 & -1 & 1 \\
E_{u} & 2 & -1 & 0 & -2 & 1 \\
\end{array}
\]

\[x^2 + y^2, z^2 \ (x^2 - y^2, \text{xy}, (xz, yz) \ (x, y) \ (x^2 - y^2, \text{xy}) \ (xz, yz) \ (x, y)]

A\(_{1g}\) always

\[\begin{align*}
&A_{1g} \\
&s \\
&d_{xy} \\
&p_{x} \\
&p_{y} \\
&p_{z} \\
&d_{xz} \\
&d_{yz} \\
&d_{x^2-y^2} \\
&d_{z^2}
\end{align*}\]