Group Theory and Symmetry

point groups, symmetry elements, matrix representations and properties of groups

2

• Name and show on a diagram five (5) symmetry elements in SF₆.
symmetry elements and associated operations

• Proper axis of Rotation
  ➤Proper rotation, $C_n$: One or more rotations by an angle of $2\pi n$ radians. The "$n$" value is often referred to as the order of the rotation axis. Note that since the bonds around the proper axis are identical, their bond moments must cancel and thus a dipole moment (if any) lies along the proper axis of rotation.

examples

• $H_2O$
• $CH_3Cl$
• $Pt(NH_3)_2Cl_2$
• $PtCl_4^{2-}$
symmetry elements and associated operations

• Plane of reflection
  ➤Reflection, $\sigma$: reflection through a plane to interchange objects on either side of the plane. Three distinct types.
  • $\sigma_v$: reflection through a plane which contains the highest order rotation axis ($C_n$ with the greatest $n$) and atoms of the molecule.
  • $\sigma_d$: similar to $\sigma_v$ but does not contain atoms of the molecule.
  • $\sigma_h$: reflection through a plane which is normal to (perpendicular to) the highest order rotation axis.

examples

• $\text{H}_2\text{O}$
• $\text{CH}_3\text{Cl}$
• $\text{cis}$ and $\text{trans}$ $\text{Pt(NH}_3)_2\text{Cl}_2$
• $\text{PtCl}_4^{2-}$
symmetry elements and associated operations

• Improper axis of rotation
  ➢ improper rotation, $S_n$: This symmetry operation consists of two consecutive operations, a proper rotation, $C_n$, followed by a horizontal reflection, $\sigma_h$.

examples

• $\text{H}_2\text{O}$
• CH$_3$Cl
• Pt(NH$_3$)$_2$Cl$_2$
• PtCl$_4^{2-}$
how to categorize molecular symmetries

- certain groups of symmetry operations form a mathematical group
- these closed sets of symmetry operations form what is called a point group

Today

- Exam is on Friday...
- HW 2 due Wednesday-solutions posted shortly after class...
- Today- point groups and matrix representations
**group work: assign point groups**

- SiCl$_3$(CH$_3$)
- trans-SF$_4$Cl$_2$
- OXeF$_4$
- CHClF$_2$
- trans-Cl$_2$C$_2$H$_2$
- CO$_2$
- PF$_3$
- cis-PtCl$_2$Br$_2$$^-$$^2$ (square planar geometry)
- cis- Cl$_2$C$_2$H$_2$
- SiClHBrF
Today’s question

• Sketch the ion $\text{PSO}_3^{3-}$ (thiophosphate) and indicate the symmetry elements present and state the point group

Up to date

• Exam Friday: quantum theory, periodicity, lewis structures and point groups are the main topics.
• Readings today...
  ➤87-100
• For Monday
  ➤109-128 (we’ll come back to vibrations... )
• Draw the symmetry elements in 1,2 dichloroethane in the *trans* configuration.

• **Closure**
  ➤ Subsequent application of any series of symmetry operations is equivalent to one of the other operations.

• **Identity**
  ➤ The do-nothing operation is important.
$$C_{2v} \text{ group multiplication table}$$

<table>
<thead>
<tr>
<th></th>
<th>$E$</th>
<th>$C_2$</th>
<th>$\sigma_v$</th>
<th>$\sigma_v'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>$E$</td>
<td>$C_2$</td>
<td>$\sigma_v$</td>
<td>$\sigma_v'$</td>
</tr>
<tr>
<td>$C_2$</td>
<td>$C_2$</td>
<td>$E$</td>
<td>$\sigma_v'$</td>
<td>$\sigma_v$</td>
</tr>
<tr>
<td>$\sigma_v$</td>
<td>$\sigma_v$</td>
<td>$\sigma_v'$</td>
<td>$E$</td>
<td>$C_2$</td>
</tr>
<tr>
<td>$\sigma_v'$</td>
<td>$\sigma_v'$</td>
<td>$\sigma_v$</td>
<td>$C_2$</td>
<td>$E$</td>
</tr>
</tbody>
</table>

matrix representations of symmetry operations

- Use the $C_{2v}$ point group as an example.
- Consider the effect of performing a $C_2$ operation on an object. The new position of a point $x,y,z$ after the operation, $x',y',z'$, can be found by using a matrix form for the operation.
- The point $x,y,z$ is found by using the three orthogonal unit vectors.
matrix representation of $C_2$ on a vector, $x, y, z$

- $C_2$ (rotation)
- $x \rightarrow -x$
- $y \rightarrow -y$
- $z \rightarrow z$
- the ‘reducible representation’ is the sum of the diagonal elements
  - $-1 + (-1) + 1 = -1$

\[
C_2 = \begin{pmatrix}
-1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

\[
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix}
= \begin{pmatrix}
-x \\
-y \\
z
\end{pmatrix}
\]

how about $\sigma_v$ on a unit vectors, $x, y, z$

- $\sigma_v$ (contains the $xz$ plane):
- $x \rightarrow x$
- $y \rightarrow -y$
- $z \rightarrow z$
- reducible representation is trace of the matrix,
  - $1 + (-1) + 1 = 1$

\[
\sigma_v = \begin{pmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

\[
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix}
= \begin{pmatrix}
x \\
-y \\
z
\end{pmatrix}
\]
\( \sigma_v' \) (contains yz plane): \( x \rightarrow -x; \ y \rightarrow y \) and \( z \rightarrow z \)

- reducible representation
  \[ \begin{align*}
  \text{reducible representation} &= -1 + 1 + 1 = 1
  \\
  \sigma_v' &= \begin{pmatrix}
  -1 & 0 & 0 \\
  0 & 1 & 0 \\
  0 & 0 & 1
  \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -x \\ y \\ z \end{pmatrix}
  \end{align*} \]

identity operation on a vector, \( x, y, z \)

- reducible representation
  \[ \begin{align*}
  \text{reducible representation} &= 1 + 1 + 1 = 3
  \\
  E &= \begin{pmatrix}
  1 & 0 & 0 \\
  0 & 1 & 0 \\
  0 & 0 & 1
  \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}
  \end{align*} \]
summarizing how (x,y,z) is transformed

- operation reducible representation
- $E$ 3
- $C_2$ -1
- $\sigma_v(xz)$ 1
- $\sigma_v(yz)$ 1
- Note that these vectors behave like the $p$ orbitals

character table for $C_{2v}$

<table>
<thead>
<tr>
<th></th>
<th>$E$</th>
<th>$C_2$</th>
<th>$\sigma_v(xz)$</th>
<th>$\sigma_v(yz)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_2$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>
• the top row which lists the symmetry operations of the point group
• the leftmost column lists the Mulliken symbols for the irreducible representations of that point group. For A and B (1 dimensional, non-degenerate irreducible representations) the difference lies in the character for the highest order rotation (for A, \( \chi = 1 \) and for B, \( \chi = -1 \)). The labels for the E and T irreducible reps can be considered arbitrarily assigned.

---

Character table for \( C_{2v} \)

<table>
<thead>
<tr>
<th></th>
<th>E</th>
<th>C2</th>
<th>( \sigma_v(xz) )</th>
<th>( \sigma_v(yz) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>A2</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>B1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>B2</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>
note several features

• number of symmetry types is equal to the number of operations
• Mullikan symbols (left column) indicate fundamental symmetry types, irreducible representations
• these are orthogonal, with cross products = 0
• These irreducible representations are analogous to unit vectors in a “symmetry space”

reducible vs. irreducible reps

• reducible representation for the vector x,y,z is not the same as any of those for the symmetry types in the character table.
• How do the individual unit vectors along the x, y and z axes transform (i.e., what are their characters)
group work: find characters for:
(no looking at books) \((C_{2v})\)

<table>
<thead>
<tr>
<th></th>
<th>E</th>
<th>C2</th>
<th>(\sigma_v(xz))</th>
<th>(\sigma_v(yz))</th>
</tr>
</thead>
<tbody>
<tr>
<td>2s</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3d(_{z^2})</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3d(_{x^2-y^2})</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3d(_{yz})</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>Rotation(x)&quot;</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>Rotation(y)</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>Rotation(z)</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
</tbody>
</table>

**Today**

- Reducible to irreducible representations
- What can be done with the irreducible representations...
- Next time: bonding theory and applications of group theory
### HE 1

<table>
<thead>
<tr>
<th>ave</th>
<th>12</th>
<th>9</th>
<th>14.3</th>
<th>10.3</th>
<th>12.3</th>
<th>54.7</th>
</tr>
</thead>
<tbody>
<tr>
<td>stddev</td>
<td>3.7</td>
<td>5.5</td>
<td>2.5</td>
<td>5.7</td>
<td>3.4</td>
<td>18.9</td>
</tr>
<tr>
<td>max</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>79.0</td>
</tr>
<tr>
<td>overall ave/q</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>11.6</td>
</tr>
</tbody>
</table>

### Character Table

<table>
<thead>
<tr>
<th>C&lt;sub&gt;2v&lt;/sub&gt;</th>
<th>E</th>
<th>C&lt;sub&gt;2&lt;/sub&gt;</th>
<th>σ&lt;sub&gt;v(xz)&lt;/sub&gt;</th>
<th>σ&lt;sub&gt;v(yz)&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>A&lt;sub&gt;1&lt;/sub&gt;</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>A&lt;sub&gt;2&lt;/sub&gt;</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>B&lt;sub&gt;1&lt;/sub&gt;</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>B&lt;sub&gt;2&lt;/sub&gt;</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>

- z, z<sup>2</sup>, x<sup>2</sup>, y<sup>2</sup>,
- R<sub>z</sub>, xy
- x, R<sub>y</sub>, xz
- y, R<sub>x</sub>, yz
symmetry of orbitals and vibrations

• how do things that are part of a molecule change under allowed symmetry operations?
• how can we determine the symmetry types of more complex systems than \((x,y,z)\)
  ➤ that is, how can one get the irreducible representations from reducible representations?

Orbitals: two methods

• by inspection
• by use of group theory and the following formula

\[
N = \frac{1}{h} \sum \chi_r^x \cdot \chi_i^x \cdot n^x
\]
add a column to character table

<table>
<thead>
<tr>
<th>$C_{2v}$</th>
<th>E</th>
<th>C2</th>
<th>$\sigma_V(xz)$</th>
<th>$\sigma_V(yz)$</th>
</tr>
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<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
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<td>1</td>
<td>-1</td>
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<td>1</td>
</tr>
</tbody>
</table>

$N = \frac{1}{h} \sum_x \chi_r^x \cdot \chi_i^x \cdot n^x$

- $N$: number of times irred rep, $x$, appears in the reducible representation
- $h$ is the order of the group (sum of all E characters)
- $\chi_r$ is the character of the reducible representation for the operation, $x$
- $\chi_i$ is the character of the irreducible representation for the operation, $x$
- $n$ is the number of operations in the class, $x$
add a column to character table

\[
\begin{array}{c|cccc|c}
C_{2v} & E & C2 & \sigma_v(xz) & \sigma_v(yz) \\
\hline
A_1 & 1 & 1 & 1 & 1 & z, z^2, x^2, y^2 \\
A_2 & 1 & 1 & -1 & -1 & R_z, xy \\
B_1 & 1 & -1 & 1 & -1 & x, R_y, xz \\
B_2 & 1 & -1 & -1 & 1 & y, R_x, yz \\
\end{array}
\]

two examples:
(x,y,z) in C_{2v}
s orbitals in PtCl_{4}^{2-} (D_{4h})

- the first example will confirm what may be deduced by inspection
- the second example will illustrate doubly degenerate irreducible representations
(x, y, z) in $C_{2v}$

- E, identity, character = 3
  
  \[
  \begin{pmatrix}
  1 & 0 & 0 \\
  0 & 1 & 0 \\
  0 & 0 & 1 \\
  \end{pmatrix}
  \begin{pmatrix}
  x \\
  y \\
  z \\
  \end{pmatrix}
  =
  \begin{pmatrix}
  x \\
  y \\
  z \\
  \end{pmatrix}
  \]

- $C_2$, proper rotation, character = -1 (note negative 1 matrix elements)
  
  \[
  C_2 = \begin{pmatrix}
  -1 & 0 & 0 \\
  0 & -1 & 0 \\
  0 & 0 & 1 \\
  \end{pmatrix}
  \begin{pmatrix}
  x \\
  y \\
  z \\
  \end{pmatrix}
  =
  \begin{pmatrix}
  -x \\
  -y \\
  z \\
  \end{pmatrix}
  \]

$\sigma_v$'s

- $\sigma_v (xz)$, character is +1 (note negative 1)
  
  \[
  \begin{pmatrix}
  1 & 0 & 0 \\
  0 & -1 & 0 \\
  0 & 0 & 1 \\
  \end{pmatrix}
  \begin{pmatrix}
  x \\
  y \\
  z \\
  \end{pmatrix}
  =
  \begin{pmatrix}
  x \\
  -y \\
  z \\
  \end{pmatrix}
  \]

- $\sigma_v (yz)$, character is +1 (note negative 1)
  
  \[
  \begin{pmatrix}
  -1 & 0 & 0 \\
  0 & 1 & 0 \\
  0 & 0 & 1 \\
  \end{pmatrix}
  \begin{pmatrix}
  x \\
  y \\
  z \\
  \end{pmatrix}
  =
  \begin{pmatrix}
  -x \\
  y \\
  z \\
  \end{pmatrix}
  \]
### Character Table for $C_{2v}$

<table>
<thead>
<tr>
<th></th>
<th>$E$</th>
<th>$C_2$</th>
<th>$\sigma_{v}(xz)$</th>
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</tr>
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<tbody>
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<td>1</td>
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<td>1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_2$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>

### Characters for Reducible Representations

- $E = 3$
- $C_2 = -1$
- $\sigma_v = 1$
- $\sigma_{v}' = 1$
\[ N = \frac{1}{h} \sum_{x} \chi_{r}^{x} \bullet \chi_{i}^{x} \bullet n^{x} \]

- \( N \): number of times irred rep, \( x \), appears in the reducible representation
- \( h \) is the order of the group (sum of all \( E \) characters)
- \( \chi_{r} \) is the character of the reducible representation for the operation, \( x \)
- \( \chi_{i} \) is the character of the irreducible representation for the operation, \( x \)
- \( n \) is the number of operations in the class, \( x \)
  - \( C_4 \) would be a class (not in \( C_{2v} \))
  - In \( C_{4v} \) there are 2 \( C_4 \)

\[ N(A_1) = \frac{1}{4} \{ 3 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 \} = 1 \]
\[ N(A_2) = \frac{1}{4} \{ 3 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 \} = 0 \]
\[ N(B_1) = \frac{1}{4} \{ 3 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 \} = 1 \]
\[ N(B_2) = \frac{1}{4} \{ 3 \cdot 1 - 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 1 \} = 1 \]
irreducible representations for $x, y, z$ in $C_{2v}$

- $A_1, B_1, B_2$

<table>
<thead>
<tr>
<th>$C_{2v}$</th>
<th>E</th>
<th>C2</th>
<th>$\sigma_v(xz)$</th>
<th>$\sigma_v(yz)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$z, z^2, x^2, y^2$</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$R_z, xy$</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$x, R_y, xz$</td>
</tr>
<tr>
<td>$B_2$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$y, R_x, yz$</td>
</tr>
</tbody>
</table>
s orbitals in PtCl$_4^{2-}$ (D$_{4h}$)

• some symmetry elements shown to right
• all the ops are listed in the table on the following slide
• need to see how the 5 orbitals transform
• know E will have red rep char = 5

character table for D$_{4h}$
use a matrix form:

\[
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
\end{pmatrix}
\begin{pmatrix}
 s_{Pt} \\
 s_{Cl1} \\
 s_{Cl2} \\
 s_{Cl3} \\
 s_{Cl4} \\
\end{pmatrix}
= 
\begin{pmatrix}
 s_{Pt} \\
 s_{Cl4} \\
 s_{Cl3} \\
 s_{Cl2} \\
 s_{Cl1} \\
\end{pmatrix}
\]

how about \( \sigma_v \)

\[
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 \\
\end{pmatrix}
\begin{pmatrix}
 s_{Pt} \\
 s_{Cl1} \\
 s_{Cl2} \\
 s_{Cl3} \\
 s_{Cl4} \\
\end{pmatrix}
= 
\begin{pmatrix}
 s_{Pt} \\
 s_{Cl1} \\
 s_{Cl4} \\
 s_{Cl3} \\
 s_{Cl2} \\
\end{pmatrix}
\]
Group work—write matrices and find the rest of the characters for the reducible representations of the Sym. Ops.

- $E$, character = 5
- $C_4$, character = 1
- $C_2$, character = 1
- $C_2'$, character = 3
- $C_2''$, character = 1
- $i$, character = 1
- $S_4$, character = 1
- $\sigma_h$, character = 5
- $\sigma_v$, character = 3
- $\sigma_d$, character = 1

$N = \frac{1}{h} \sum_x \chi_r^x \cdot \chi_i^x \cdot n^x$

- $N$: number of times irred rep, $x$, appears in the reducible representation
- $h$ is the order of the group (sum of all $E$ characters)
- $\chi_r$ is the character of the reducible representation for the operation, $x$
- $\chi_i$ is the character of the irreducible representation for the operation, $x$
- $n$ is the number of operations in the class, $x$
now to find irred reps in the reducible representation

\[ h = 1 + 2 + 1 + 2 + 2 + 1 + 2 + 1 + 2 + 2 = 16 \]

\[ N(A_{1g}) = \frac{1}{16} \{ 1 \cdot 5 \cdot 1 + 1 \cdot 1 \cdot 2 + 1 \cdot 1 \cdot 1 + 1 \cdot 3 \cdot 2 + 1 \cdot 1 \cdot 2 + 1 \cdot 1 \cdot 1 + 1 \cdot 1 + 1 \cdot 5 \cdot 1 + 1 \cdot 3 \cdot 2 + 1 \cdot 1 \cdot 2 \} \]

\[ N(A_{1g}) = 2 \]

\[ N(A_{2g}) = \frac{1}{16} \{ 1 \cdot 5 \cdot 1 + 1 \cdot 1 \cdot 2 + 1 \cdot 1 \cdot 1 + (-1 \cdot 3 \cdot 2) + (-1 \cdot 1 \cdot 2) + 1 \cdot 1 \cdot 1 + 1 \cdot 1 \cdot 1 + 1 \cdot 5 \cdot 1 + (-1 \cdot 3 \cdot 2) + (-1 \cdot 1 \cdot 2) \} = 0 \]

\[ N(B_{1g}) = \frac{1}{16} \{ 1 \cdot 5 \cdot 1 + (-1 \cdot 1 \cdot 2) + 1 \cdot 1 \cdot 1 + 1 \cdot 3 \cdot 2 + 1 \cdot 1 \cdot 2 + (-1 \cdot 1 \cdot 1) + (-1 \cdot 1 \cdot 1) + 1 \cdot 5 \cdot 1 + (1 \cdot 3 \cdot 2) + (-1 \cdot 1 \cdot 2) \} = 1 \]

\[ N(B_{2g}) = 0 \]

\[ N(E_g) = \frac{1}{16} \{ 2 \cdot 5 \cdot 1 + (0 \cdot 1 \cdot 2) + (-2 \cdot 1 \cdot 1) + 0 \cdot 3 \cdot 2 + 0 \cdot 1 \cdot 2 + (2 \cdot 1 \cdot 1) + 0 \cdot 1 \cdot 1) + (-2 \cdot 5 \cdot 1 + (0 \cdot 3 \cdot 2) + (0 \cdot 1 \cdot 2) \} = 0 \]
finally

- $N(A_{1u}) = 1/16$
- $\{1\cdot5\cdot1+(1\cdot1\cdot2)+1\cdot1\cdot1+1\cdot3\cdot2+1\cdot1\cdot2+(-1\cdot1\cdot1)+(-1\cdot1\cdot1)+(-1\cdot5\cdot1)+(-1\cdot3\cdot2)+(-1\cdot1\cdot2)\} = 0$
- $N(A_{2u}) = 0$
- $N(B_{1u}) = 0$
- $N(B_{2u}) = 0$
- $N(E_u) = 1$

irreducible representations are

- 2 $A_{1g}$ irreducible reps
- 1 $B_{1g}$ irreducible rep
- 1 $E_u$ irred rep
  ➢ the $E_u$ rep is 2 fold degenerate (identity character is 2)
  ➢ indicates that some “s” orbitals are interchanged under the symmetry operations of the $D_{4h}$ point group
irreducible representations are useful

- used in determination of molecular orbitals
  - orbitals that combine must be of same symmetry
- used in determining allowed transitions
  - symmetries of vibrations are important
  - use vectors to describe motion