<table>
<thead>
<tr>
<th>Element</th>
<th>Operation</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>E, the identity</td>
<td>Does nothing</td>
<td>All objects posses E</td>
</tr>
<tr>
<td>$C_n$, n-fold rotation</td>
<td>• Rotate object by $2\pi/n$ about the n-fold axis.</td>
<td>• $\text{H}_2\text{O}$ posses a $C_2$ axis</td>
</tr>
<tr>
<td></td>
<td>• The axis with the highest n is called the principle axis.</td>
<td>• $\text{NH}_3$ posses a $C_3$ axis</td>
</tr>
<tr>
<td></td>
<td>• For n&gt;2 the sense is important…$C_n^+$ - clockwise rotation…$C_n^-$-counterclockwise rotation</td>
<td>• Benzene posses a $C_2$, $C_3$, $C_6$, and two sets of three $C_2$ axes perpendicular to the $C_6$ axis</td>
</tr>
<tr>
<td>$\sigma$, reflection plane</td>
<td><strong>Reflects through the plane</strong></td>
<td>Three types</td>
</tr>
<tr>
<td>$\sigma_v$, vertical plane</td>
<td>Plane containing the principle axis</td>
<td>• $\text{H}_2\text{O}$</td>
</tr>
<tr>
<td>$\sigma_h$, horizontal plane</td>
<td>Plane perpendicular to the principle axis</td>
<td>• Benzene</td>
</tr>
<tr>
<td>$\sigma_d$, dihedral plane</td>
<td>Vertical plane which bisects two $C_2$ axes perpendicular to the principal axis</td>
<td>• Benzene</td>
</tr>
<tr>
<td>i, inversion center</td>
<td>Sends each atom through the origin along a straight line so that $x\rightarrow-x$, $y\rightarrow-y$, and $z\rightarrow-z$</td>
<td>• $\text{H}_2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• $\text{CO}_2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Benzene</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• $\text{SF}_6$</td>
</tr>
<tr>
<td>$S_n$, n-fold improper rotation axis</td>
<td>Rotate object by $2\pi/n$, then reflects through plane perpendicular to the axis of rotation</td>
<td>• $\text{CH}_4$</td>
</tr>
</tbody>
</table>
Let’s take the ECLIPSED conformation of ethane

- One three-fold axis coincident with the C-C bond
- Three two-fold axes perpendicular to the C-C bond and intersecting its midpoint
- Three reflection planes, each containing the C-C bond and a pair of C-H bonds
- One reflection plane perpendicular to the C-C bond and bisecting it
- NO CENTER OF INVERSION IS PRESENT
- One three-fold *improper* axis coincident with the C-C bond
Let’s take the STAGGERED conformation of ethane

- One three fold axis coincident with the C-C bond
- Three two-fold axes perpendicular to the C-C bond and intersecting its midpoint
- Three reflection planes, each containing the C-C bond and a pair of C-H bond
- No reflection plane perpendicular to the C-C bond…we lost it!
- One point of inversion at the midpoint of the C-C bond…we gained it!
- One six-fold improper axis coincident with the C-C bond…changed its order!
Stereographic Projections

Working Area

General Point
Let's consider the symmetry elements of the $C_{2v}$ point group and the resulting symmetry operations.
Still considering the symmetry elements of the $C_{2v}$ point group and the resulting symmetry operations.
Let’s compare our results with the $C_{2v}$ character table...

$$\sigma_v \cdot \sigma_v' = E$$

$$C_2 \cdot \sigma_v = \sigma_v'$$

$$\sigma_v \cdot \sigma_v = C_2$$
Lets try this with another point group and build the character table…

<table>
<thead>
<tr>
<th></th>
<th>$C_{2h}$</th>
<th>E</th>
<th>$C_2$</th>
<th>$\sigma_h$</th>
<th>$i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_2$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\sigma_h$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$i$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
$i \rightarrow E$

$E \cdot i = i$

$C_2 \cdot i = \sigma_h$

$\sigma_h \cdot i = C_2$

$i \cdot i = E$
This gives us the following for the Character Table…

<table>
<thead>
<tr>
<th>$C_{2h}$</th>
<th>$E$</th>
<th>$C_2$</th>
<th>$\sigma_h$</th>
<th>$i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td></td>
<td></td>
<td></td>
<td>$i$</td>
</tr>
<tr>
<td>$C_2$</td>
<td></td>
<td></td>
<td>$\sigma_h$</td>
<td></td>
</tr>
<tr>
<td>$\sigma_h$</td>
<td></td>
<td></td>
<td></td>
<td>$C_2$</td>
</tr>
<tr>
<td>$i$</td>
<td></td>
<td></td>
<td></td>
<td>$E$</td>
</tr>
</tbody>
</table>

Complete the rest as we have done and hand it in on Tuesday
Point Groups

• Symmetry operations may be organized into groups that obey the four properties of mathematical groups…namely…

1. There exists an identity operator that commutes with all other members
2. The product of any two members must also be a member
3. Multiplication is associative
4. The existence of an inverse for each member

• It will be possible to assign ANY molecule to one of these so-called Point Groups
  ➢ So named because the symmetry operation leaves one point unchanged
• Point Group $C_1$
  ➢ Trivial group with contains all molecules having no symmetry
  ➢ There is no center of inversion, plane of reflection, improper axis of rotation, etc.
  ➢ The molecule HNCIF (below) is such a molecule
Point Groups

• Point Group $C_s$
  ➢ Only molecules which have to them a plane of reflection as a symmetry element
  ➢ Formyl Chloride belongs to this point group

```
H
\ \\  
C=O
 \ \ \ 
Cl
```
Point Groups

- **Point Group $C_i$**
  - Molecules whose sole symmetry element is an inversion center
  - As an example take the rotamer of 1,2-dichloro-1,2-difluoroethane in which the fluorine atoms are off-set to one another
  - The only operations generated by this inversion are $i$ and $i^2=E$...this is a group of order 2 and is designated $C_i$

*Important to note that $i$ is the same as an $S_2$ axis*
Point Groups

• Point Group $C_n$
  ➢ Molecules with only an n-fold axis of rotation
  ➢ Boric acid with the hydrogen atoms lying above the BO$_3$ plane is an example
• **Point Group $C_{nv}$**

  - Molecules with an $n$-fold $C_n$ axis of rotation and $n$ vertical mirror planes which are colinear with the $C_n$ axis
  - Water belongs to such a point group…the $C_{2v}$

  Note that if you find a $C_n$ axis and one $\sigma_v$ plane then you are guaranteed to find $n$ $\sigma_v$ planes
Point Groups

• **Point Group $C_{nh}$**
  - This point group is generated by a $C_n$ axis of rotation AND a *horizontal* mirror plane, $\sigma_h$, which is *perpendicular* to the $C_n$ axis.
  - Trans-butadiene (trans-1,3-butene) is an example of the $C_{2h}$ point group.
• **Point Group Dₙ**
  - This point group is generated by a Cₙ axis of rotation and a C₂ axis which is *perpendicular* to the Cₙ axis...no mirror planes
  - Tris(ethylenediamine)cobalt(III) possesses idealized D₃ symmetry

*Build this molecule and convince yourself that this is indeed the case!!*
Point Groups

• **Point Group $D_{nd}$**
  ➢ This point group is generated by a $C_n$ axis of rotation and a $C_2$ axis which is *perpendicular* to the $C_n$ axis and a dihedral mirror plane, $\sigma_d$.
  ➢ The dihedral plane is colinear with the principal axis and bisects the perpendicular $C_2$ axis.
  ➢ Crystals of $\text{Cs}_2\text{CuCl}_4$ have a squashed tetrahedral $D_{2d}$ structure.
Point Groups

• Point Group $D_{nh}$
  ➢ This point group is generated by a $C_n$ axis of rotation and $n$ $C_2$ axis which is *perpendicular* to the $C_n$ axis and a horizontal mirror plane which is by definition *perpendicular* to the **principal axis of rotation**
  ➢ Benzene is the classic example, possessing $D_{6h}$ symmetry
Point Groups

- Point Groups $S_n$
  - These point groups are generated by an $S_n$ axis.
  - For example, the spirononane...tetraflourospironononane belongs to the $S_4$ point group and only elements generated by $S_4$
    - $S_4$
    - $S_4^2 = C_2$
    - $S_4^3$
    - $S_4^4 = E$
  - The $S_2$ point group is just $C_1$ since $S_2 = i$
  - When $n$ is odd the point groups are just the same as the $C_{nh}$ point groups and so are designated as such
    - As a direct result, only $S_4$, $S_6$, and $S_8$, ...have a separate existence
Special Point Groups

- Tetrahedral molecules belong to the point group $T_d$
- Octahedral molecules belong to the point group $O_h$
- Molecules with icosahedral (20 triangular faces) or dodecahedral (12 pentagonal faces) belong to the point group $I_h$
- Atoms…which have spherical symmetry, belong to the point group $K_h$
- The point group $T_h$, which may be obtained by adding to $T_d$ as set of $\sigma_h$ planes, which contain pairs of $C_2$ axis…as opposed to the $\sigma_d$ planes which contain one $C_2$ axis and bisect another pair, giving $T_d$)