Practice:
Your turn, please determine the number of times the $E'$ and $A_1''$ irreducible representations contribute to the reducible representation of $H_3$.

<table>
<thead>
<tr>
<th></th>
<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>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1''$</td>
<td></td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$\Gamma(H_3)$</td>
<td></td>
<td>3</td>
<td>0</td>
<td>1</td>
<td>3</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

$$n_{A_1''} = \frac{1}{12} \left( 1 \cdot 1 \cdot 3 \right) + \left( 2 \cdot 1 \cdot 0 \right) + \left( 3 \cdot 1 \cdot 1 \right) + \left( 1 \cdot -1 \cdot 3 \right) + \left( 2 \cdot -1 \cdot 0 \right) + \left( 3 \cdot -1 \cdot 1 \right) = 0$$

$$n_{A_1''} = \frac{1}{12} \left[ 3 + 0 + 3 - 3 + 0 - 3 \right] = 0$$

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<tbody>
<tr>
<td>$E'$</td>
<td></td>
<td>2</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>-1</td>
<td>0</td>
</tr>
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</tr>
</tbody>
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$$n_{E'} = \frac{1}{12} \left( 2 \cdot 1 \cdot 3 \right) + \left( 2 \cdot -1 \cdot 0 \right) + \left( 3 \cdot 0 \cdot 1 \right) + \left( 2 \cdot 1 \cdot 3 \right) + \left( 2 \cdot -1 \cdot 0 \right) + \left( 3 \cdot 0 \cdot 1 \right) = \frac{12}{12} = 1$$

$$n_{E'} = \frac{1}{12} \left( 6 + 0 + 0 + 6 + 0 + 0 \right) = \frac{12}{12} = 1$$
Degenerate fragment orbitals

• producing the two wavefunctions for the degenerate fragment orbitals is slightly more difficult, but we start in exactly the same way, first produce a projection table for the E’ irreducible representation:

\[
\begin{array}{cccccccc}
Q[s_i] & s_1 & s_2 & s_3 & s_1 & s_3 & s_2 & s_1 & s_3 & s_2 \\
E' & 2 & -1 & -1 & 0 & 0 & 0 & 2 & -1 & -1 & 0 & 0 & 0 \\
\chi_e'(Q) \cdot Q \cdot [s_i] & 2s_1 & -s_2 & -s_3 & - & - & 2s_1 & -s_2 & -s_3 & - & - & - \\
\end{array}
\]

The e’ projection table

• Then form the sum of these entries to determine the equation of the first orbital contributing to the degenerate pair:

\[
P_{E'}[s_i] = \frac{1}{12} \left[ 2s_1 - s_2 - s_3 + 2s_1 - s_2 - s_3 \right]
\]

\[
P_{E'}[s_i] = \frac{1}{12} \left[ 4s_1 - 2s_2 - 2s_3 \right] = \frac{1}{6} \left[ 2s_1 - s_2 - s_3 \right]
\]

\[
\psi_{e'} = \frac{1}{6} \left[ 2\phi_{s_1} - \phi_{s_2} - \phi_{s_3} \right]
\]

One of the e’ fragment orbitals of H₃

• when drawing the orbitals be careful to make the correct phase and size assignments, so orbital s₁ is twice as large as s₂ or s₃ and has a positive phase, while s₂ and s₃ have negative phase. Which orbital is s₁, s₂ or s₃ is determined by the initial labelling of the system.