Hexagonal $D_6 \subset D_{6h}$ and octahedral-tetrahedral $O\sim T_d$ symmetry

(Int.J.Mol.Sci, 14, 714(2013) p.755-774 , QTCA Unit 5 Ch. 15 )
(PSDS - Ch. 4 )

Review: Symmetry reduction and splitting: Subduced irep $D^\alpha(D_3)\downarrow C_2 = d^{02} \oplus d^{12} \oplus \ldots$ correlation
Symmetry induction and clustering: Induced rep $d^a(C_2)\uparrow D_3 = D^\alpha \oplus D^\beta \oplus \ldots$ correlation

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$D_3$-$C_2$ Coset structure of $d^{m_2}(C_2)\uparrow D_3$ induced representation basis
$D_3$-Projection of $d^{m_2}(C_2)\uparrow D_3$ induced representation basis
Derivation of Frobenius reciprocity

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry
Irreducible characters
Irreducible representations
Correlations with $D_6$ characters:
...and $C_2(i_3)$ characters......and $C_6(1,h^1,h^2,...)$ characters
$D_6$ symmetry and induced representation band structure

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B-Type Symmetry Breaking

Bilateral subgroup
Chain $D_3 \supset C_2$

Subduced irep $D_\alpha(D_3) \downarrow C_2$
B-Type Symmetry Breaking

Bilateral subgroup
Chain $D_3 \supset C_2$
(or $C_{3v} \supset C_v$)

Subduced irep $D^\alpha(D_3) \downarrow C_2$
Applied symmetry reduction and splitting: Subduced irep $D^\alpha(D_3) \downarrow C_2 = d^{02} \oplus d^{12} \oplus \ldots$ correlation

<table>
<thead>
<tr>
<th>$D_3 \supseteq C_2$</th>
<th>0_2</th>
<th>1_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
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<tr>
<td>$A_2$</td>
<td>.</td>
<td>1</td>
</tr>
<tr>
<td>$E_1$</td>
<td>1</td>
<td>1</td>
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</table>

$D^{A_1}(D_3) \downarrow C_2 \sim d^{02}$
$D^{A_2}(D_3) \downarrow C_2 \sim d^{12}$
$D^{E_1}(D_3) \downarrow C_2 \sim d^{02} \oplus d^{12}$

Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = g|I\rangle$ of position ket $|g\rangle$
Applied symmetry reduction and splitting: Subduced irrep \( D^\alpha(D_3) \downarrow C_2 = d^{02} \oplus d^{12} \oplus \ldots \) correlation

<table>
<thead>
<tr>
<th>( D_3 \supset C_2 )</th>
<th>( \omega^\alpha ) relabel/split</th>
<th>( \omega^\alpha ) relabel/reduce</th>
<th>( \omega^\alpha ) relabel/split</th>
<th>( D_3 \supset C_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_1 )</td>
<td>( P^A = P^A P^{02} = P^{A}_{0,02} )</td>
<td>( D^A \downarrow C_2 \sim d^{02} )</td>
<td>( \Rightarrow \omega^A \rightarrow \omega^{02} )</td>
<td>( A_1 )</td>
</tr>
<tr>
<td>( A_2 )</td>
<td>( P^A = P^A P^{12} = P^{A}_{1,12} )</td>
<td>( D^A \downarrow C_2 \sim d^{12} )</td>
<td>( \Rightarrow \omega^A \rightarrow \omega^{12} )</td>
<td>( A_2 )</td>
</tr>
<tr>
<td>( E_1 )</td>
<td>( P^E = P^E P^{02} + P^E P^{12} = P^E_{0,02} + P^E_{1,12} )</td>
<td>( D^E \downarrow C_2 \sim d^{02} \oplus d^{12} )</td>
<td>( \Rightarrow \omega^E \rightarrow \omega^{02} )</td>
<td>( E_1 )</td>
</tr>
</tbody>
</table>

\( \Rightarrow C_2 \)

<table>
<thead>
<tr>
<th>( D_3 )</th>
<th>( 1 ) { ( r^1, r^2 ) } { i_1, i_3 }</th>
<th>( 0 ) { ( r^1, r^2 ) } { i_1, i_3 }</th>
<th>( 1 ) { ( r^1, r^2 ) } { i_1, i_3 }</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_1 )</td>
<td>1 1 1</td>
<td>1 1 1</td>
<td></td>
</tr>
<tr>
<td>( A_2 )</td>
<td>1 1 -1</td>
<td>1 1 -1</td>
<td></td>
</tr>
<tr>
<td>( E_1 )</td>
<td>2 -1 0</td>
<td>1 -1 0</td>
<td></td>
</tr>
</tbody>
</table>

\( D^A(D_3) \downarrow C_2 \sim d^{02} \)
\( D^A(D_3) \downarrow C_2 \sim d^{12} \)
\( D^E(D_3) \downarrow C_2 \sim d^{02} \oplus d^{12} \)

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Introduction to octahedral tetrahedral symmetry $O_h \supset O\sim T_d \supset T$
Applied symmetry reduction and splitting: Subduced irrep $D^\alpha(D_3) \downarrow C_2 = d^{02} \oplus d^{12} \oplus \ldots$ correlation

<table>
<thead>
<tr>
<th>$D_3 \supset C_2$</th>
<th>$\mathbf{P}^\alpha$ relabel/split</th>
<th>$D^\alpha$ relabel/reduce</th>
<th>$\omega^\alpha$ relabel/split</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>$\mathbf{P}^A_1 = \mathbf{P}^A \mathbf{P}^{02} = \mathbf{P}^A_{0,02}$</td>
<td>$\Rightarrow D^A \downarrow C_2 \sim d^{02}$</td>
<td>$\Rightarrow \omega^A_1 \rightarrow \omega^{02}$</td>
</tr>
<tr>
<td>$A_2$</td>
<td>$\mathbf{P}^A_2 = \mathbf{P}^A \mathbf{P}^{l_2} = \mathbf{P}^A_{l_2}$</td>
<td>$\Rightarrow D^A \downarrow C_2 \sim d^{12}$</td>
<td>$\Rightarrow \omega^A_2 \rightarrow \omega^{12}$</td>
</tr>
<tr>
<td>$E_1$</td>
<td>$\mathbf{P}^{E_1} = \mathbf{P}^{E_1} \mathbf{P}^{02} + \mathbf{P}^{E_1} \mathbf{P}^{l_2}$</td>
<td>$\Rightarrow D^E_1 \downarrow C_2 \sim d^{02} \oplus d^{12}$</td>
<td>$\Rightarrow \omega^{E_1} \rightarrow \omega^{02}$</td>
</tr>
</tbody>
</table>

Spontaneous symmetry breaking and clustering:
Induced rep $d^a(C_2)^\uparrow D_3 = D^\alpha \oplus D^\beta \oplus \ldots$ correlation

<table>
<thead>
<tr>
<th>$D_3 \supset C_2$</th>
<th>0 2 1 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1 1</td>
</tr>
<tr>
<td>$E_1$</td>
<td>1 1</td>
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Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = g|1\rangle$ of position ket $|g\rangle$

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C-Type Symmetry Breaking

Trigonal subgroup
Chain $D_3 \supset C_3$
(or $C_{3v} \supset C_3$)

Subduced irrep $D^a(D_3) \downarrow C_3$
**Applied symmetry reduction and splitting:** Subduced rep $D^\alpha(D_3)\downarrow C_2 = d_{02} \oplus d_{12} \oplus \ldots$ correlation

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<th>$\omega^\alpha$ relabel/split</th>
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<tr>
<td>$A_1$</td>
<td>$\mathbf{P}<em>A = \mathbf{P} \cdot \mathbf{P}</em>{02}$</td>
<td>$\Rightarrow D_A \downarrow C_2 \sim d_{02}$</td>
<td>$\Rightarrow \omega_A \rightarrow \omega_{02}$</td>
</tr>
<tr>
<td>$A_2$</td>
<td>$\mathbf{P}<em>A = \mathbf{P} \cdot \mathbf{P}</em>{12}$</td>
<td>$\Rightarrow D_A \downarrow C_2 \sim d_{12}$</td>
<td>$\Rightarrow \omega_A \rightarrow \omega_{12}$</td>
</tr>
<tr>
<td>$E_1$</td>
<td>$\mathbf{P}<em>E = \mathbf{P} \cdot \mathbf{P}</em>{02} + \mathbf{P} \cdot \mathbf{P}_{12}$</td>
<td>$\Rightarrow D_E \downarrow C_2 \sim \omega$</td>
<td>$\Rightarrow \omega_E \rightarrow \omega_{02}$</td>
</tr>
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</table>

$\Rightarrow C_2$ relabel/split

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<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>.</td>
</tr>
<tr>
<td>$A_2$</td>
<td>.</td>
<td>1</td>
</tr>
<tr>
<td>$E_1$</td>
<td>1</td>
<td>1</td>
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</tbody>
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Spontaneous symmetry breaking and clustering: Induced rep $d^a(C_2)\uparrow D_3 = D^\alpha \oplus D^\beta \oplus \ldots$ correlation

<table>
<thead>
<tr>
<th>$D_3 \supset C_3$</th>
<th>$1 = r^0$</th>
<th>$r^1$</th>
<th>$r^2 = r^j$</th>
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</thead>
<tbody>
<tr>
<td>$(0)_2$</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$(1)_2$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$(+1)_3$</td>
<td>1</td>
<td>$\varepsilon$</td>
<td>$\varepsilon^*$</td>
</tr>
<tr>
<td>$(0)_3$</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$(2)_3 = (-1)_3$</td>
<td>1</td>
<td>$\varepsilon^*$</td>
<td>$\varepsilon$</td>
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</tbody>
</table>
Spontaneous symmetry breaking and clustering: 
Induced rep $\alpha(C_2) \uparrow D_3 = \alpha \oplus \beta \oplus \ldots$ correlation

$D_3 \supseteq C_2$

<table>
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<tr>
<th>$D^e$ relabel/reduce</th>
<th>$\omega^e$ relabel/split</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D^e \downarrow C_2 \sim d_{02}$</td>
<td>$\omega^e \rightarrow \omega^0$</td>
</tr>
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</table>

$A_1$

$P_A^e = P_A^* P_0^{02} = P_{A_1}^{02}$

$\Rightarrow D^A \downarrow C_2 \sim d_{02}$

$\Rightarrow \omega^A \rightarrow \omega_{02}$

$A_2$

$P_A^e = P_A^* P_1^{12} = P_{A_1}^{12}$

$\Rightarrow D^A \downarrow C_2 \sim d_{12}$

$\Rightarrow \omega^A \rightarrow \omega_{12}$

$E_1$

$P_E^e = P_E^* P_0^{02} + P_E^* P_1^{12}$

$\Rightarrow D^E \downarrow C_2 \sim d_{02} \oplus d_{12}$

$\Rightarrow \omega^E \rightarrow \omega^0 \oplus \omega^1$

Applied symmetry reduction and splitting: Subduced rep $D^\alpha(D_3) \downarrow C_2 = d_{02} \oplus d_{12} \oplus \ldots$ correlation

$\Rightarrow C_2$

<table>
<thead>
<tr>
<th>$\Rightarrow C_3$</th>
<th>1</th>
<th>$r'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$E_1$</td>
<td>2</td>
<td>0</td>
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$D_3 \supseteq C_3$

<table>
<thead>
<tr>
<th>$D_3 \supseteq C_3$</th>
<th>0</th>
<th>1</th>
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<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>\cdot</td>
</tr>
<tr>
<td>$A_2$</td>
<td>\cdot</td>
<td>1</td>
</tr>
<tr>
<td>$E_1$</td>
<td>\cdot</td>
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$D^A_1(D_3) \downarrow C_3 \sim d_{02}$

$D^A_2(D_3) \downarrow C_3 \sim d_{12}$

$D^E_1(D_3) \downarrow C_3 \sim d_{02} \oplus d_{12}$

$\Rightarrow C_3$

<table>
<thead>
<tr>
<th>$\Rightarrow C_3$</th>
<th>1=r^0</th>
<th>$r'$</th>
<th>$r^2=r^1$</th>
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<tbody>
<tr>
<td>(0)</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>(1)</td>
<td>1</td>
<td>-1</td>
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$D^A_1(D_3) \downarrow C_3 \sim d_{02}$

$D^A_2(D_3) \downarrow C_3 \sim d_{12}$

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<td>1</td>
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<td>$\varepsilon^*$</td>
</tr>
<tr>
<td>(2)</td>
<td>1</td>
<td>$\varepsilon^*$</td>
<td>$\varepsilon$</td>
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$D^A_1(D_3) \downarrow C_3 \sim d_{02}$

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<tr>
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<td>$A_1$</td>
<td>$\mathbf{P}^A = \mathbf{P}^A \mathbf{P}^{02} = \mathbf{P}^{A_{02}}$</td>
<td>$\Rightarrow D^A \downarrow C_2 \sim d^{02}$</td>
<td>$\Rightarrow \omega^A \rightarrow \omega^{02}$</td>
<td>$A_1$</td>
<td>1 _1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>$\mathbf{P}^A = \mathbf{P}^A \mathbf{P}^{03} = \mathbf{P}^{A_{03}}$</td>
<td>$\Rightarrow D^A \downarrow C_2 \sim d^{03}$</td>
<td>$\Rightarrow \omega^A \rightarrow \omega^{03}$</td>
<td>$A_2$</td>
<td>_1 _1</td>
</tr>
<tr>
<td>$E_1$</td>
<td>$\mathbf{P}^E = \mathbf{P}^E \mathbf{P}^{02} + \mathbf{P}^E \mathbf{P}^{03}$</td>
<td>$\Rightarrow D^E \downarrow C_2 \sim$</td>
<td>$\Rightarrow \omega^E \rightarrow \omega^{02}$</td>
<td>$E_1$</td>
<td>1 _1</td>
</tr>
</tbody>
</table>

Spontaneous symmetry breaking and clustering:
Induced rep $d^\alpha(C_2) \uparrow D_3 = D^\alpha \oplus D^\beta \oplus \ldots$ correlation

\[
\begin{array}{ccc}
\alpha & \beta & \gamma \\
1 & 1 & 1 \\
0 & 1 & 1 \\
1 & 0 & 1 \\
1 & 1 & 0 \\
\end{array}
\]

Applied symmetry reduction and splitting: Subduced irep $D^\alpha(D_3) \downarrow C_3 = d^{03} \oplus d^{13} \oplus \ldots$ correlation

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<td>$A_1$</td>
<td>$\mathbf{P}^A = \mathbf{P}^A \mathbf{P}^{03} = \mathbf{P}^{A_{03}}$</td>
<td>$\Rightarrow D^A \downarrow C_3 \sim d^{03}$</td>
<td>$\Rightarrow \omega^A \rightarrow \omega^{03}$</td>
<td>$A_1$</td>
<td>1 _1 _1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>$\mathbf{P}^A = \mathbf{P}^A \mathbf{P}^{03} = \mathbf{P}^{A_{03}}$</td>
<td>$\Rightarrow D^A \downarrow C_3 \sim d^{03}$</td>
<td>$\Rightarrow \omega^A \rightarrow \omega^{03}$</td>
<td>$A_2$</td>
<td>1 _1 _1</td>
</tr>
<tr>
<td>$E_1$</td>
<td>$\mathbf{P}^E = \mathbf{P}^E \mathbf{P}^{02} + \mathbf{P}^E \mathbf{P}^{03}$</td>
<td>$\Rightarrow D^E \downarrow C_2 \sim$</td>
<td>$\Rightarrow \omega^E \rightarrow \omega^{13} \oplus \omega^{23}$</td>
<td>$E_1$</td>
<td>_1 _1 _1</td>
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$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry
Irreducible characters
Irreducible representations
Correlations with $D_6$ characters:
...and $C_2(i_3)$ characters......and $C_6(1, h^1, h^2, \ldots)$ characters
$D_6$ symmetry and induced representation band structure

Introduction to octahedral tetrahedral symmetry $O_h \supset O \supset T_d \supset T$
Applied symmetry reduction and splitting: Subduced irep \(D^\alpha(D_3)\downarrow C_2 = d^{02} \oplus d^{12} \oplus \ldots \) correlation

<table>
<thead>
<tr>
<th>(D_3 \supset C_2)</th>
<th>(\mathbf{P}^\alpha) relabel/split</th>
<th>(D^\alpha) relabel/reduce</th>
<th>(\omega^\alpha) relabel/split</th>
<th>(D_3 \supset C_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A_1)</td>
<td>(\mathbf{P}^A = \mathbf{P}^0 = \mathbf{P}^0_{02})</td>
<td>(\Rightarrow D^A \downarrow C_2 \sim d^{02})</td>
<td>(\Rightarrow \omega^A \rightarrow \omega^{02})</td>
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<tr>
<td>(A_2)</td>
<td>(\mathbf{P}^B = \mathbf{P}^1 = \mathbf{P}^0_{12})</td>
<td>(\Rightarrow D^A \downarrow C_2 \sim d^{12})</td>
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</tr>
<tr>
<td>(E_1)</td>
<td>(\mathbf{P}^E = \mathbf{P}^E_1 + \mathbf{P}^E_2)</td>
<td>(\Rightarrow D^E_1 \downarrow C_2 \sim \omega^{02})</td>
<td>(\Rightarrow \omega^E \rightarrow \omega^{02})</td>
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</table>

Spontaneous symmetry breaking and clustering: Induced rep \(d^\alpha(C_2)\uparrow D_3 = D^\alpha \oplus D^\beta \oplus \ldots \) correlation

\[
\begin{array}{|c|c|c|c|}
\hline
D_3 & 1 & \{r'^1, r'^2\} & \{i_1, i_2, i_3\} \\
\hline
A_1 & 1 & 1 & 1 \\
A_2 & 1 & 1 & -1 \\
E_1 & 2 & -1 & 0 \\
\hline
\end{array}
\]

Applied symmetry reduction and splitting: Subduced irep \(D^\alpha(D_3)\downarrow C_3 = d^{03} \oplus d^{13} \oplus \ldots \) correlation

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<td>(\mathbf{P}^E = \mathbf{P}^E_1 + \mathbf{P}^E_2)</td>
<td>(\Rightarrow D^E_1 \downarrow C_3 \sim \omega^{03})</td>
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</tr>
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Spontaneous symmetry breaking and clustering: Induced rep \(d^\alpha(C_3)\uparrow D_3 = D^\alpha \oplus D^\beta \oplus \ldots \) correlation

\[
\begin{array}{|c|c|c|}
\hline
\supset C_3 & 1 & r' \quad r' \quad r'^2 = r'^2 \\
\hline
(0)_2 & 1 & 1 & 1 \\
(1)_2 & 1 & \varepsilon & \varepsilon^* \\
(2)_{2} = (-1)_3 & 1 & \varepsilon^* & \varepsilon \\
\hline
\end{array}
\]
Review: Symmetry reduction and splitting: Subduced irep $D^\alpha(D_3) \downarrow C_2 = d_0^2 \oplus d_1^2 \oplus \ldots$ correlation
Symmetry induction and clustering: Induced rep $d^\alpha(C_2) \uparrow D_3 = D^\alpha \oplus D^\beta \oplus \ldots$ correlation

$D_3 - C_2$ Coset structure of $d^m_2(C_2) \uparrow D_3$ induced representation basis
$D_3$ - Projection of $d^m_2(C_2) \uparrow D_3$ induced representation basis
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Introduction to octahedral tetrahedral symmetry $O_h \supseteq O \supseteq T_d \supseteq T$
$D_3 - C_2$ Coset structure of $d_{m2}(C_2)^\uparrow D^3$ induced representation basis

Left cosets $[1C_2 = (1, i_3), \ r^1C_2 = (r^1, i_2), \ r^2C_2 = (r^2, i_1)]$ relate to sets of $r^p$-transformed kets.
D₃-C₂ Coset structure of d³m₂(C₂)↑D₃ induced representation basis

Left cosets \[ [1C₂ = (1, i_3), \quad r¹C₂ = (r¹, i_2), \quad r²C₂ = (r², i_1)] \]

\[ [1(|1\rangle, |i_3\rangle) = (|1\rangle, |i_3\rangle), \quad r¹(|1\rangle, |i_3\rangle) = (|r¹\rangle, |i_2\rangle), \quad r²(|1\rangle, |i_3\rangle) = (|r²\rangle, |i_1\rangle)] \]
Left cosets \([1C_2 = (1, i_3), \quad \textbf{r}^1C_2 = (\textbf{r}^1, i_2), \quad \textbf{r}^2C_2 = (\textbf{r}^2, i_1)]\) relate to sets of \(\textbf{r}^p\)-transformed kets

\[
[1(\textbf{1}, i_i)] = (\textbf{1}, i_i), \quad \textbf{r}^1(1, i_i)] = (\textbf{r}^1, i_2), \quad \textbf{r}^2(1, i_i)] = (\textbf{r}^2, i_1)]
\]

Right cosets \([C_2 = (1, i_3), \quad \textbf{C}_2 \textbf{r}^2 = (\textbf{r}^2, i_2), \quad \textbf{C}_2 \textbf{r} = (\textbf{r}, i_1)]\) relate to sets of bras

\[
[A(\textbf{1}, i_i)] = (A, i_i), \quad \textbf{A}^1(1, i_i)] = (\textbf{A}^1, i_2), \quad \textbf{A}^2(1, i_i)] = (\textbf{A}^2, i_1)]
\]
**D₃-C₂ Coset structure of \( d^{m_2}(C_2) \uparrow D^3 \)**

**Left cosets** \([1C_2 = (1, i_3), \ r^1C_2 = (r^1, i_2), \ r^2C_2 = (r^2, i_1)]\) relate to sets of \( r^p \)-transformed kets

\[ ([1(|1\rangle, |i_3\rangle) = (|1\rangle, |i_3\rangle), \ r^1(|1\rangle, |i_3\rangle) = (|r^1\rangle, |i_2\rangle), \ r^2(|1\rangle, |i_3\rangle) = (|r^2\rangle, |i_1\rangle)] \]

**Right cosets** \([C_2=(1, i_3), \ C_2r^2=(r^2, i_2), \ C_2r=(r, i_1)]\) relate to sets of bras

\[ ([\langle 1 |, \langle i_3 |) 1 = (\langle 1 |, \langle i_3 |), \ \langle 1 |, \langle i_3 |) r^2 = (\langle r^1 |, \langle i_2 |), \ \langle 1 |, \langle i_3 |) r^1 = (\langle r^2 |, \langle i_1 |)] \]
**D₃-C₂ Coset structure of dₘ²(C₂)↑D³ induced representation basis**

Left cosets $[1C₂ = (1, i₃), \quad r¹C₂ = (r¹, i₂), \quad r²C₂ = (r², i₁)]$ relate to sets of $r^p$-transformed kets

$$[1(|1⟩, |i₃⟩) = (|1⟩, |i₃⟩), \quad r¹(|1⟩, |i₃⟩) = (|r¹⟩, |i₂⟩), \quad r²(|1⟩, |i₃⟩) = (|r²⟩, |i₁⟩)]$$

Right cosets $[C₂ = (1, i₃), \quad C₂r² = (r², i₂), \quad C₂r = (r, i₁)]$ relate to sets of bras

$$[(⟨1|, ⟨i₃|)1 = (⟨1|, ⟨i₃|), \quad (⟨1|, ⟨i₃|)r² = (⟨r¹|, ⟨i₂|), \quad (⟨1|, ⟨i₃|)r† = (⟨r²|, ⟨i₁|)]$$

C₂ projectors $P^{0₂} = \frac{1}{2}(1 + i₃) = P^x$ and $P^{1₂} = \frac{1}{2}(1 - i₃) = P^y$ split ket $|r⟩ = r|1⟩$ or bra $⟨r| = ⟨1|r^†$ into ± coset sums
Left cosets \[ [1 C_2 = (1, i_3), \quad r^1 C_2 = (r^1, i_2), \quad r^2 C_2 = (r^2, i_1)] \] relate to sets of \( r^p \)-transformed kets

\[ [1(\langle 1 | l i_3 \rangle ) = (\langle 1 | l i_3 \rangle ), \quad r^1(\langle 1 | l i_3 \rangle ) = (\langle r^1 | l i_2 \rangle ), \quad r^2(\langle 1 | l i_3 \rangle ) = (\langle r^2 | l i_1 \rangle )] \]

Right cosets \[ [C_2 = (1, i_3), \quad C_2 r^2 = (r^2, i_2), \quad C_2 r = (r, i_1)] \] relate to sets of bras

\[ [(\langle 1 | l i_3 \rangle ) 1 = (\langle 1 | l i_3 \rangle ), \quad (\langle 1 | l i_3 \rangle ) r^2 = (\langle r^1 | l i_2 \rangle ), \quad (\langle 1 | l i_3 \rangle ) r^1 = (\langle r^2 | l i_1 \rangle )] \]

\( C_2 \) projectors \( P^{02} = \frac{1}{2} (1 + i_3) = P^x \) and \( P^{12} = \frac{1}{2} (1 - i_3) = P^y \) split ket \( |r\rangle = |1\rangle \) or bra \( \langle r| = \langle 1| \) into \( \pm \) coset sums

\[
\begin{bmatrix}
P^{n_2}|1\rangle = \frac{1}{2}(|1\rangle \pm |i_3\rangle), \\
|n\rangle = |r^{0}\rangle, \\
|n\rangle = |r^{1}\rangle,
\end{bmatrix}
\text{basis of } d^{n_2} \uparrow D_3
**D₃-C₂ Coset structure of D⁻¹(C₂) \uparrow D³ induced representation basis**

*Left cosets* \([1C₂ = (1, i₃), \quad r¹C₂ = (r¹, i₂), \quad r²C₂ = (r², i₁)]\) relate to sets of \(r^p\)-transformed kets

\[ [1(1, i₃)] = (1, i₃), \quad r¹(1, i₃)] = (r¹, i₂), \quad r²(1, i₃)] = (r², i₁)\]

*Right cosets* \([C₂ = (1, i₃), \quad C₂r² = (r², i₂), \quad C₂r = (r, i₁)]\) relate to sets of bras

\[ [(1, i₃)₁ = (1, i₃)₁, \quad (1, i₃)₁r² = (r¹, i₂)₁, \quad (1, i₃)₁r¹ = (r², i₁)₁]\]

\(\mathbb{C}_2\) projectors \(\mathbb{P}^0₂ = \frac{1}{2}(1 + i₃) = P^x\) and \(\mathbb{P}^1₂ = \frac{1}{2}(1 - i₃) = P^y\) split ket \(\mid r\rangle = \mid r\rangle \mid 1\rangle\) or bra \(\langle r\mid = \langle r\mid 1\rangle^\dagger\) into ± coset sums

\[
\begin{align*}
\mathbb{P}^n₂\mid 1\rangle &= \frac{1}{2}(\mid 1\rangle ± \mid i₃\rangle), \\
\langle 1\mid \mathbb{P}^n₂ &= \frac{1}{2}(\langle 1\rangle ± \langle i₃\rangle),
\end{align*}
\]

\[
\begin{bmatrix}
\mathbb{P}^n₂\mid 1\rangle \\
\langle 1\mid \mathbb{P}^n₂
\end{bmatrix} =
\begin{bmatrix}
\mid rₙ\rangle \\
\langle rₙ\rangle
\end{bmatrix}, \quad \text{basis of } D⁻¹₂ \uparrow D₃
\]

\[
\begin{bmatrix}
\mathbb{P}^n₂\mid 1\rangle \\
\langle 1\mid \mathbb{P}^n₂
\end{bmatrix} =
\begin{bmatrix}
\mid rₙ\rangle \\
\langle rₙ\rangle
\end{bmatrix}, \quad \text{basis of } D⁻¹₂ \uparrow D₃
\]

Tuesday, March 31, 2015
**Review:** Symmetry reduction and splitting: Subduced irep $D^α(D_3)\downarrow C_2 = d^{02} \oplus d^{12} \oplus \ldots$ correlation
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**D₃-C₂ Coset structure of d^{m_2}(C₂)↑D³ induced representation basis**

**Left cosets** \([1C₂ = (1, i₃), \quad r^1C₂ = (r^1, i₂), \quad r^2C₂ = (r^2, i₁)]\) relate to sets of \(r^p\)-transformed kets

\[\begin{align*}
[1(1), i₃)) &= (1, i₃)), & r^1(1), i₃)) &= (r^1, i₂)), & r^2(1), i₃)) &= (r^2, i₁))
\end{align*}\]

**Right cosets** \([C₂=(1, i₃), C₂r^2=(r^2, i₂), C₂r=(r, i₁)]\) relate to sets of bras

\[\begin{align*}
[(1, i₃)|1 &= ([1, i₃)), & (1, i₃)|r^2 &= ([r^1, i₂)), & (1, i₃)|r^1 &= ([r^2, i₁])
\end{align*}\]

\(C₂\) projectors \(P^{02} = \frac{1}{2}(1+i₃) = P^x\) and \(P^{12} = \frac{1}{2}(1-i₃) = P^y\) split ket \(|r⟩= r|1⟩\) or bra \(⟨r| = ⟨1|r^†⟩\) into ± coset sums

\[
\begin{bmatrix}
P^{n2}|1⟩ = \frac{1}{2}(|1⟩ ± |i₃⟩), \\
⟨1|P^{n2} = \frac{1}{2}(⟨1⟩ ± ⟨i₃⟩),
\end{bmatrix}
\]

\(\sigma\)-bond" ket

\[
\begin{bmatrix}
|r^0⟩, |r^1⟩, |r^2⟩
\end{bmatrix}
\]

of induced rep. \(d^{n_2}↑D₃\)

\(|r^0⟩ = |0^\dot{0}_2x⟩\)

\(|r^0⟩ + |i₃⟩)/\sqrt{2}\)

\(r^0\) basis of \(d^{n_2}↑D₃\)

\(r^0\) basis of \(d^{n_2}↑D₃\)
**D₃-C₂ Coset structure of dₘ₂(C₂)↑D₃ induced representation basis**

**Left cosets** \([1C₂ = (1, i₃), \quad r^1C₂ = (r^1, i₂), \quad r^2C₂ = (r^2, i₁)]\) relate to sets of \(r^p\)-transformed kets

\[
[1(l₁, l₃)] = (l₁, l₃), \quad r^1(l₁, l₃) = (l₁, r₁l₂), \quad r^2(l₁, l₃) = (l₂, r₂l₁)
\]

**Right cosets** \([C₂ = (1, i₃), \quad C₂r^2 = (r², i₂), \quad C₂r = (r, i₁)]\) relate to sets of bras

\[
[(l₁, l₃)] = (l₁, l₃), \quad (l₁, l₃)r² = (l₁, r₂l₁), \quad (l₁, l₃)r^1 = (l₂, r₁l₂)
\]

\(C₂\) projectors \(P_{0²}^{0} = \frac{1}{2}(1 + i₃) = P^x\) and \(P_{1²}^{1} = \frac{1}{2}(1 - i₃) = P^y\) split ket \((r) = r|1\rangle\) or bra \(|r\rangle = |1\rangle r^\dagger\) into ± coset sums

\[
\begin{align*}
P_{0²}^{0} |1\rangle &= \frac{1}{2} (|1\rangle \pm |i₃\rangle), \\
\langle 1|P_{0²}^{0} &= \frac{1}{2} (\langle 1| \pm \langle i₃|),
\end{align*}
\]

**"σ-bond" ket**

\[
\left[ |r^0_x\rangle, |r^1_x\rangle, |r^2_x\rangle \right]
\]

of induced rep. \(d^{0²}↑D₃\)

**"π-bond" ket**

\[
\left[ |r^0_y\rangle, |r^1_y\rangle, |r^2_y\rangle \right]
\]

of induced rep. \(d^{1²}↑D₃\)
**D₃-C₂ Coset structure of \(d_{m_2}(C_2) \uparrow D³\) induced representation basis**

Left cosets \([1C₂ = (1, i₃), \quad r^1C₂ = (r^1, i₂), \quad r^2C₂ = (r^2, i₁)]\) relate to sets of \(r^p\)-transformed kets

\[
\begin{align*}
[1(1\mid i₃)] & = (1\mid i₃), \quad r^1(1\mid i₃) = (r^1\mid i₂), \quad r^2(1\mid i₃) = (r^2\mid i₁)
\end{align*}
\]

Right cosets \([C₂ = (1, i₃), \quad C₂r² = (r², i₂), \quad C₂r² = (r, i₁)]\) relate to sets of bras

\[
\begin{align*}
[(\langle 1\mid i₃ \rangle \mid 1) & = (\langle 1\mid i₃ \rangle \mid 1), \quad (\langle 1\mid i₃ \rangle \mid r²) = (\langle r^1\mid i₂ \rangle \mid 1), \quad (\langle 1\mid i₃ \rangle \mid r²) = (\langle r^2\mid i₁ \rangle \mid 1)
\end{align*}
\]

\(C₂\) projectors \(P^{i₃} = \frac{1}{2}(1 + i₃) = P^x\) and \(P^{i₂} = \frac{1}{2}(1 - i₃) = P^y\) split ket \(r = r^1\mid 1\rangle\) or bra \(\langle r = 1\mid r^{\dagger}\rangle\) into ± coset sums

\[
\begin{align*}
\langle r^1\mid P^{i₂} = \frac{1}{2} \langle r^1\mid i₂ \rangle \\
\langle r^1\mid P^{i₃} = \frac{1}{2} \langle r^1\mid i₃ \rangle
\end{align*}
\]

"\(\sigma\)-bond" ket

\[
\begin{align*}
|1_{x}^{\uparrow\downarrow}\rangle = |0_{2_{x}}^{\uparrow\downarrow}\rangle = \sqrt{2}(\mid r^1\rangle + \mid i₂\rangle)
\end{align*}
\]

de of induced rep. \(d_{m_2} \uparrow D₃\)

"\(\pi\)-bond" ket

\[
\begin{align*}
|1_{y}^{\uparrow\downarrow}\rangle = |0_{2_{y}}^{\uparrow\downarrow}\rangle = \sqrt{2}(\mid r^1\rangle - \mid i₂\rangle)
\end{align*}
\]

de of induced rep. \(d_{m_2} \uparrow D₃\)

Tuesday, March 31, 2015
$D_3$-$C_2$ Coset structure of $d^{m_2}(C_2)^\uparrow D^3$ induced representation basis

Left cosets $[1C_2 = (1, i_3), \quad r^1 C_2 = (r^1, i_2), \quad r^2 C_2 = (r^2, i_1)]$ relate to sets of $r^p$-transformed kets

$$[1(1, i_3)) = (11, i_3)), \quad r^1(1, i_3)) = (r^1, i_2)), \quad r^2(1, i_3)) = (r^2, i_1))]$$

Right cosets $[C_2=(1, i_3), \quad C_2 r^2=(r^2, i_2), \quad C_2 r=(r, i_1)]$ relate to sets of bras

$$[(1, i_3) 1 = (1, i_3), \quad (1, i_3) r^2 = (r^1, i_2), \quad (1, i_3) r^t = (r^2, i_1)]$$

$C_2$ projectors $P^{02}=\frac{1}{2}(1+i_3)=P^x$ and $P^{12}=\frac{1}{2}(1-i_3)=P^y$ split ket $\langle r|r 1 \rangle$ or bra $\langle r|=\langle 1| r^t$ into $\pm$ coset sums

$$[\begin{array}{c}
\langle r^2 |P^{n2} = \frac{1}{2}(r^2 \pm i_1) \\
\langle r^2 |P^{n2} = \frac{1}{2}(r^2 \pm i_1)
\end{array}$$

basis of $d^{n_2} \uparrow D_3$

"$\sigma$-bond" ket

$$[|r^0_x\rangle, |r^1_x\rangle, |r^2_x\rangle]$$

of induced rep. $d^{0_2} \uparrow D_3$

"$\pi$-bond" ket

$$[|r^0_y\rangle, |r^1_y\rangle, |r^2_y\rangle]$$

of induced rep. $d^{1_2} \uparrow D_3$
**D₃-C₂ Coset structure of \(d_{m2}(C₂)^{\uparrow D^3}\) induced representation basis**

Left cosets \([1C₂ = (1, i₂), \quad r^1C₂ = (r^1, i₂), \quad r^2C₂ = (r^2, i₂)]\) relate to sets of \(r^p\)-transformed kets

\[
[1(1)|i₃\rangle) = (1)|i₃\rangle, \quad r^1(1)|i₃\rangle) = (r^1)|i₂\rangle, \quad r^2(1)|i₃\rangle) = (r^2)|i₁\rangle)
\]

Right cosets \([C₂ = (1, i₃), \quad C₂r² = (r², i₂), \quad C₂r = (r, i₁)]\) relate to sets of bras

\[
[(<1, i₃>)|1) = (<1, i₃>)|1), \quad (<1, i₃>)|r²) = (<r^1, i₂>)|1), \quad (<1, i₃>)|r) = (<r², i₁>)|1)]
\]

\(C₂\) projectors \(P^{02} = \frac{1}{2}(1 + i₃) = P^x\) and \(P^{12} = \frac{1}{2}(1 - i₃) = P^y\) split ket \(|r⟩ = |1⟩\) or bra \(⟨r| = ⟨1|r^†\) into ± coset sums

\[
\Big[ P^{n2}_{n2} |1⟩ = \frac{1}{2}(|1⟩ ± |i₃⟩), \quad P^{n2}_{n2} |r^1⟩ = \frac{1}{2}(|r^1⟩ ± |i₂⟩), \quad P^{n2}_{n2} |r²⟩ = \frac{1}{2}(|r²⟩ ± |i₁⟩) \Big] = \Big[ |r^0⟩, |r^1⟩, |r²⟩ \Big] \] basis of \(d^{n2} \uparrow D_3\)

\[
\Big[ ⟨1|P^{n2}_{n2} = \frac{1}{2}(⟨1| ± ⟨i₃|), \quad ⟨r^1|P^{n2}_{n2} = \frac{1}{2}(⟨r^1| ± ⟨i₂|), \quad ⟨r²|P^{n2}_{n2} = \frac{1}{2}(⟨r²| ± ⟨i₁|) \Big] = \Big[ ⟨r^0|, ⟨r^1|, ⟨r²| \Big] \] basis of \(d^{n2} \uparrow D_3\)

3 "σ-bond" kets

\[
|r^1_x⟩ = |0^1_{2x}⟩
= (|r^1⟩ + |i₂⟩)/\sqrt{2}
\]

\(d^0_{x} \uparrow D_3\)

3 "π-bond" kets

\[
|r^0_y⟩ = |1^0_{2y}⟩
= (|r^0⟩ - |i₃⟩)/\sqrt{2}
\]

\(d^1_{z} \uparrow D_3\)
Review: Symmetry reduction and splitting: Subduced irep $D^\alpha(D_3) \downarrow C_2 = d^{02} \oplus d^{12} \oplus \ldots$ correlation
Symmetry induction and clustering: Induced rep $d^a(C_2) \uparrow D_3 = D^\alpha \oplus D^\beta \oplus \ldots$ correlation

$D_3\times C_2$ Coset structure of $d^{m_2}(C_2) \uparrow D_3$ induced representation basis
$D_3$-Projection of $d^{m_2}(C_2) \uparrow D_3$ induced representation basis
Derivation of Frobenius reciprocity

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry
Irreducible characters
Irreducible representations
Correlations with $D_6$ characters:
...and $C_2(i_3)$ characters......and $C_6(1, h^1, h^2, \ldots)$ characters
$D_6$ symmetry and induced representation band structure

Introduction to octahedral tetrahedral symmetry $O_h \supset O \sim T_d \supset T$
**D3-Projection of \(d^{m_2}(C_2)^\uparrow D_3\) induced representation basis**

\(D_3 \supseteq C_2\) projectors \(P_{A_1}^{0_20_2}, P_{A_2}^{0_20_2}, P_{E_1}^{0_20_2}, P_{E_1}^{0_21_2}, P_{E_1}^{1_20_2}, P_{E_1}^{1_21_2}\) must reduce induced representation \(d^{m_2}(C_2)^\uparrow D_3\)

---

\(\sigma\)-bond ket

\[
\begin{bmatrix}
|r_x^0\rangle, |r_x^1\rangle, |r_x^2\rangle
\end{bmatrix}
\]

of induced rep. \(d^{0_2}_x \uparrow D_3\)

\[|r_x^0\rangle = |0_{2_1}^{A_0} x\rangle\]

\[= (|r_x^0\rangle + |i_3\rangle)/\sqrt{2}\]
"σ-bond" ket
\[
\begin{bmatrix}
| r_x^0 \rangle \\
| r_x^1 \rangle \\
| r_x^2 \rangle
\end{bmatrix}
\]
of induced rep.
\[d_{0z}^0 \Uparrow D_3\]

But, which \(D_3\) projector \(P_{j_2k_2}^\mu\) will work on base \(| r_{m_2}^0 \rangle = p_{m_2}^\mu | 1 \rangle\) of induced representation \(d_{m_2}^m (C_2) \Uparrow D_3\)
$D_3$-$C_2$ Coset structure of $d^{m_2}(C_2) \uparrow D^3$ induced representation basis

$D_3 \supseteq C_2$ projectors $\mathbf{P}^{A_1}_{0202}, \mathbf{P}^{A_2}_{1212}, \mathbf{P}^{E_1}_{0202}, \mathbf{P}^{E_1}_{0212}, \mathbf{P}^{E_1}_{1202}, \mathbf{P}^{E_1}_{1212}$ must reduce induced representation $d^{m_2}(C_2) \uparrow D_3$

But, which $D_3$ projector $\mathbf{P}^\mu_{j_2k_2}$ will work on base $|r^0_{m_2}\rangle = \mathbf{p}^{m_2} |1\rangle$ of induced representation $d^{m_2}(C_2) \uparrow D_3$

$$\mathbf{P}^\mu_{j_2k_2} |r^0_{m_2}\rangle = \mathbf{P}^\mu_{j_2k_2} \mathbf{p}^{m_2} |1\rangle = ?$$
**D\textsubscript{3}-C\textsubscript{2} Coset structure of \(d\textsuperscript{m\textsubscript{2}}(C\textsubscript{2}) \uparrow D\textsuperscript{3}\) induced representation basis**

\(D\textsubscript{3}\supset C\textsubscript{2}\) projectors \(P_{0202}^{A_1}, P_{1212}^{A_2}, P_{0202}^{E_1}, P_{0212}^{E_1}, P_{1202}^{E_1}, P_{1212}^{E_1}\) must reduce induced representation \(d\textsuperscript{m\textsubscript{2}}(C\textsubscript{2}) \uparrow D\textsubscript{3}\).

**But, which \(D\textsubscript{3}\) projector \(P^\mu_{j_2k_2}\) will work on base \(|r\textsubscript{m\textsubscript{2}}^0\rangle = p\textsuperscript{m\textsubscript{2}}|1\rangle\) of induced representation \(d\textsuperscript{m\textsubscript{2}}(C\textsubscript{2}) \uparrow D\textsubscript{3}\)?**

\[
P^\mu_{j_2k_2}|r\textsubscript{m\textsubscript{2}}^0\rangle = P^\mu_{j_2k_2}p\textsuperscript{m\textsubscript{2}}|1\rangle = \delta\textsuperscript{m\textsubscript{2}}_{k_2}P^\mu_{j_2m\textsubscript{2}}|1\rangle
\]

Local symmetry \(k_2\) of \(P^\mu_{j_2k_2}\) must match that of \(|r\textsubscript{m\textsubscript{2}}^0\rangle\).

---

"\(\sigma\)-bond" ket
\[
\begin{bmatrix}
| r\textsubscript{x}^0\rangle, | r\textsubscript{x}^1\rangle, | r\textsubscript{x}^2\rangle
\end{bmatrix}
\]
of induced rep.
\(d\textsuperscript{0\textsubscript{2}x} \uparrow D\textsubscript{3}\)

\[| r\textsubscript{x}^0\rangle = |0\textsubscript{2x}^\textsuperscript{A0}\rangle \]
\[=(| r\textsubscript{0}\rangle + | i\textsubscript{3}\rangle)/\sqrt{2} \]
\[ \text{D}_3-\text{C}_2 \text{ Coset structure of } d^{m_2}(\text{C}_2) \uparrow \text{D}_3 \text{ induced representation basis} \]

\[ \text{D}_3 \supseteq \text{C}_2 \text{ projectors } P_{0_2 0_2}^{A_1}, P_{1_2 1_2}^{A_2}, P_{0_2 0_2}^{E_1}, P_{0_2 1_2}^{E_1}, P_{1_2 0_2}^{E_1} \text{ must reduce induced representation } d^{m_2}(\text{C}_2) \uparrow \text{D}_3 \]

But, which \( D_3 \) projector \( P_{j_2 k_2}^{\mu} \) will work on base \( \left| r_{m_2}^0 \right\rangle = p_{m_2}^{0^2} \left| 1 \right\rangle \) of induced representation \( d^{m_2}(\text{C}_2) \uparrow \text{D}_3 \)

\[ P_{j_2 k_2}^{\mu} \left| r_{m_2}^0 \right\rangle = P_{j_2 k_2}^{\mu} p_{m_2}^{0^2} \left| 1 \right\rangle = \delta_{m_2}^0 P_{j_2 m_2}^{\mu} \left| 1 \right\rangle \]

Local symmetry \( k_2 \) of \( P_{j_2 k_2}^{\mu} \) must match that \( m_2 \) of \( \left| r_{m_2}^0 \right\rangle \)

For example, base \( \left| r_{x}^0 \right\rangle = \left| r_{0_2}^0 \right\rangle = p_{0_2}^{0^2} \left| 1 \right\rangle \) of \( d^{0^2}(\text{C}_2) \uparrow \text{D}_3 \) gives zero for all \( P_{j_2 k_2}^{\mu} \) except \( P_{0_2 0_2}^{A_1}, P_{0_2 0_2}^{E_1}, \) and \( P_{1_2 0_2}^{E_1} \),

\( D_3 \) projectors: \( P_{0_2 0_2}^{A_1}, P_{1_2 1_2}^{A_2}, P_{0_2 0_2}^{E_1}, P_{0_2 1_2}^{E_1}, P_{1_2 0_2}^{E_1} \).

\( C_2 \{0_2, 1_2\} \) Notation

"\( \sigma \)-bond" ket
\[ \left[ \left| r_{x}^0 \right\rangle, \left| r_{y}^1 \right\rangle, \left| r_{z}^2 \right\rangle \right] \]
of induced rep.
\( d^{0^2} \uparrow \text{D}_3 \)

\[ \left| r_{x}^0 \right\rangle = \left| 0_2^A 0 \right\rangle \]
\[ \left| r_{x} \right\rangle = (\left| r_{y}^0 \right\rangle + \left| i_{3} \right\rangle)/\sqrt{2} \]

\( Tuesday, March 31, 2015 \)
**$D_3$-$C_2$ Coset structure of $d^{m_2}(C_2) \uparrow D^3$ induced representation basis**

$D_3 \supseteq C_2$ projectors $P_{0_20_2}^{A_1}, P_{1_21_2}^{A_1}, P_{0_20_2}^{E_1}, P_{0_21_2}^{E_1}, P_{1_20_2}^{E_1}, P_{1_21_2}^{E_1}$ must reduce induced representation $d^{m_2}(C_2) \uparrow D_3$

**But, which $D_3$ projector $P_{j_2 k_2}^{\mu}$ will work on base $| r_{m_2}^0 \rangle = P_{m_2}^{0} | 1 \rangle$ of induced representation $d^{m_2}(C_2) \uparrow D_3$**

$$P_{j_2 k_2}^{\mu} | r_{m_2}^0 \rangle = P_{j_2 k_2}^{\mu} P_{m_2}^{0} | 1 \rangle = \delta_{k_2}^{m_2} P_{j_2 m_2}^{\mu} | 1 \rangle$$

Local symmetry $k_2$ of $P_{j_2 k_2}^{\mu}$ must match that $m_2$ of $| r_{m_2}^0 \rangle$

For example, base $| r_x^0 \rangle = | r_{0_2}^0 \rangle = P_{0_2}^0 | 1 \rangle$ of $d^{0_2}(C_2) \uparrow D_3$ gives zero for all $P_{j_2 k_2}^{\mu}$ except $P_{0_20_2}^{A_1}, P_{0_20_2}^{E_1}, P_{1_20_2}^{E_1}$.

**$D_3$ projectors:** $P_{0_21_2}^{A_1}, P_{1_21_2}^{A_1}, P_{0_20_2}^{E_1}, P_{0_21_2}^{E_1}, P_{1_20_2}^{E_1}$

**$C_2$ projectors:** $P_{x}^{A_1}, P_{y}^{A_1}, P_{x}^{E_1}, P_{y}^{E_1}, P_{xy}^{E_1}, P_{x}^{E_1}, P_{y}^{E_1}, P_{xy}^{E_1}$

"$\sigma$-bond" ket

$$\left[ | r_x^0 \rangle, | r_y^0 \rangle, | r_{x+y}^0 \rangle \right]$$

of induced rep. $d^{0_2} \uparrow D_3$

These give the “$x$-band”
D3-C2 Coset structure of $d^{m_2}(C_2) \uparrow D^3$ induced representation basis

$D_3 \supseteq C_2$ projectors $P_{0202}^{A_1}, P_{1212}^{A_2}, P_{0202}^{E_1}, P_{0212}^{E_1}, P_{1202}^{E_1}, P_{1212}^{E_1}$ must reduce induced representation $d^{m_2}(C_2) \uparrow D_3$

But, which $D_3$ projector $P_{j_2 k_2}^{\mu}$ will work on base $r_{m_2}^0 = p^m_2 |1\rangle$ of induced representation $d^{m_2}(C_2) \uparrow D_3$

$P_{j_2 k_2}^{\mu} |r_{m_2}^0\rangle = P_{j_2 k_2}^{\mu} p^m_2 |1\rangle = \delta_{k_2}^{m_2} P_{j_2 m_2}^{\mu} |1\rangle$

Local symmetry $k_2$ of $P_{j_2 k_2}^{\mu}$ must match that $m_2$ of $r_{m_2}^0$

For example, base $|r_{x}^0\rangle = |r_{02}^0\rangle = p^0_2 |1\rangle$ of $d^0_2(C_2) \uparrow D_3$ gives zero for all $P_{j_2 k_2}^{\mu}$ except $P_{0202}^{A_1}, P_{0202}^{E_1},$ and $P_{1202}^{E_1}$,

$D_3$ projectors: $P_{0202}^{A_1}, P_{1212}^{A_2}, P_{0202}^{E_1}, P_{0212}^{E_1}, P_{1202}^{E_1}, P_{1212}^{E_1}$

$C_2 \{0, 1\}$ Notation $\{x, y\}$ Notation $P_{xx}^{A_1}, P_{xy}^{A_2}, P_{xy}^{E_1}, P_{xx}^{E_1}, P_{xy}^{E_1}, P_{yy}^{E_1}$

"$\pi$-bond" ket $[|r_{y}^0\rangle, |r_{y}^1\rangle, |r_{y}^2\rangle]$ of induced rep. $d^1_2 \uparrow D_3$

These give the "$y$-band"
Frobenius Reciprocity Theorem for $G \supset K$

Number of $D^\alpha$ in $d^k(K) \uparrow G = \text{Number of } d^k \text{ in } D^\alpha(G) \downarrow K$
Frobenius Reciprocity Theorem for \( G \supset K \)

Number of \( D^\alpha \) in \( d^k(K) \uparrow G \) = Number of \( d^k \) in \( D^\alpha(G) \downarrow K \)

.. applies to regular representation

\[
\begin{array}{c|c}
D_3 \supset C_1 & 0_1 = 1_1 \\
\hline
A_1 & 1 \\
A_2 & 1 \\
E_1 & 2 \\
\end{array}
\]
Frobenius Reciprocity Theorem for \( G \supset K \)

Number of \( D^\alpha \) in \( d^K (K) \uparrow G \) = Number of \( d^K \) in \( D^\alpha (G) \downarrow K \)

..applies to regular representation

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<td>( A_2 )</td>
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<tr>
<td>( E_1 )</td>
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..and other induced representations

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<td>( E_1 )</td>
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$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry
**Irreducible characters**
**Irreducible representations**
**Correlations with $D_6$ characters:**
...and $C_2(i_3)$ characters......and $C_6(1,h^1,h^2,...)$ characters
$D_6$ symmetry and induced representation band structure

**Introduction to octahedral tetrahedral symmetry $O_h \supset O \sim T_d \supset T$**
**Bilateral subgroup**

**Chain** \(D_6 \supset D_3 \supset C_2\)
Bilateral subgroup

Chain $D_{6h} \supset D_6 \supset D_3 \supset C_2$

(To be studied later)
$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry

$D_6$ is the outer product ($\times$) product $D_3 \times C_2$ of $D_3$ and $C_2$. (Requires $C_2$ to commute with all of $D_3$.)

$D_6 = D_3 \times C_2 = \{1, r, r^2, i_1, i_2, i_3\} \times \{1, R_z\}$
$D_6 \supseteq D_2 \supseteq C_2 = D_3 \times C_2$ symmetry and outer product geometry

$D_6$ is the outer product ($\times$) product $D_3 \times C_2$ of $D_3$ and $C_2$. (Requires $C_2$ to commute with all of $D_3$.)

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× product and $D_6$ operators. Define hexagonal generator $h(60^\circ)$ of subgroup $C_6 = \{1, h, h^2, h^3, h^4, h^5\}$

$D_6 = D_3 \times C_2 = \{1, r, r^2, i_1, i_2, i_3, 1 \cdot R_z, r \cdot R_z, r^2 \cdot R_z, i_1 \cdot R_z, i_2 \cdot R_z, i_3 \cdot R_z\}$
$D_6 \supseteq D_2 \supseteq C_2 = D_3 \times C_2$ symmetry and outer product geometry

$D_6$ is the outer product ($\times$) product $D_3 \times C_2$ of $D_3$ and $C_2$. (Requires $C_2$ to commute with all of $D_3$.)

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$\times$ product and $D_6$ operators. Define hexagonal generator $h_{(60^\circ)}$ of subgroup $C_6 = \{1, h, h^2, h^3, h^4, h^5\}$

$D_6 = D_3 \times C_2 = \{1, r, r^2, i_1, i_2, i_3, 1 \cdot R_z, r \cdot R_z, r^2 \cdot R_z, i_1 \cdot R_z, i_2 \cdot R_z, i_3 \cdot R_z\}$

$D_6 = D_3 \times C_2 = \{1, h^2, h^4, i_1, i_2, i_3, h^3, h^5, h, j_1, j_2, j_3\}$
\( D_6 \supset D_2 \supset C_2 = D_3 \times C_2 \) symmetry and outer product geometry

\( D_6 \) is the outer product \((\times)\) product \( D_3 \times C_2 \) of \( D_3 \) and \( C_2 \). (Requires \( C_2 \) to commute with all of \( D_3 \).)

\( D_6 = D_3 \times C_2 = \{1, r, r^2, i_1, i_2, i_3\} \times \{1, R_z\} \)

\( \times \) product and \( D_6 \) operators. Define hexagonal generator \( h_{(60^\circ)} \) of subgroup \( C_6 = \{1, h, h^2, h^3, h^4, h^5\} \)

\[ D_6 = D_3 \times C_2 = \{1, r, r^2, i_1, i_2, i_3, 1 \cdot R_z, r \cdot R_z, r^2 \cdot R_z, i_1 \cdot R_z, i_2 \cdot R_z, i_3 \cdot R_z\} \]

\[ D_6 = D_3 \times C_2 = \{1, h^2, h^4, i_1, i_2, i_3, h^3, h^5, h, j_1, j_2, j_3\} \]

Note: \( h^2 = r_{(120^\circ)} \) and \( h^3 = R_z(180^\circ) \) and \( h^4 = r^2 \) and \( h^5 = r \cdot R_z \)
$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry

$D_6$ is the outer product (×) product $D_3 \times C_2$ of $D_3$ and $C_2$. (Requires $C_2$ to commute with all of $D_3$.)

$D_6 = D_3 \times C_2 = \{1, r, r^2, i_1, i_2, i_3\} \times \{1, R_z\}$

× product and $D_6$ operators. Define hexagonal generator $h_{(60^\circ)}$ of subgroup $C_6 = \{1, h, h^2, h^3, h^4, h^5\}$

$D_6 = D_3 \times C_2 = \{1, r, r^2, i_1, i_2, i_3, 1 \cdot R_z, r \cdot R_z, r^2 \cdot R_z, i_1 \cdot R_z, i_2 \cdot R_z, i_3 \cdot R_z\}$

$D_6 = D_3 \times C_2 = \{1, h^2, h^4, i_1, i_2, i_3, h^3, h^5, h, j_1, j_2, j_3\}$

Note: $h^2 = r_{(120^\circ)}$ and $h^3 = R_z_{(180^\circ)}$ and $h^4 = r^2$ and $h^5 = r \cdot R_z$

Electrostatic potential $V(\phi)$ doesn't care which way is "up." Wells remain wells, and barriers remain barriers under all $D_6$ operations.

NOTE:
The $i_a$ and $j_b$ do not flip over the potential plot.
Review: Symmetry reduction and splitting: Subduced rep \(D^\alpha(D_3)\downarrow C_2 = d_0^2 \oplus d_2^{12} \oplus \ldots\) correlation
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Introduction to octahedral tetrahedral symmetry \(O_h \supset O \sim T_d \supset T\)
$$D_6 \supset D_2 \supseteq C_2 = D_3 \times C_2$$

Irreducible characters

| $D_3$ | 1 \{r, r^2\} \{i_1, i_2, i_3\} |
|---|---|---|
| $\chi^A_1 (g)$ | 1 | 1 | 1 |
| $\chi^A_2 (g)$ | 1 | 1 | -1 |
| $\chi^E_1 (g)$ | 2 | -1 | 0 |

\[
\begin{array}{c|ccc|ccc|ccc}
   & D_3 \times C_2^Z & 1 \{r, r^2\} & \{i_1, i_2, i_3\} & 1 \cdot R_z & \{r, r^2\} \cdot R_z & \{i_1, i_2, i_3\} \cdot R_z \\
\hline
A_1 \cdot (A) & 1 \cdot 1 & 1 \cdot 1 & 1 \cdot 1 & 1 \cdot 1 & 1 \cdot 1 & 1 \cdot 1 \\
A_2 \cdot (A) & 1 \cdot 1 & 1 \cdot 1 & -1 \cdot 1 & 1 \cdot 1 & 1 \cdot 1 & -1 \cdot 1 \\
E_1 \cdot (A) & 2 \cdot 1 & -1 \cdot 1 & 0 \cdot 1 & 2 \cdot 1 & -1 \cdot 1 & 0 \cdot 1 \\
A_1 \cdot (B) & 1 \cdot 1 & 1 \cdot 1 & 1 \cdot 1 & 1 \cdot (-1) & 1 \cdot (-1) & 1 \cdot (-1) \\
A_2 \cdot (B) & 1 \cdot 1 & 1 \cdot 1 & -1 \cdot 1 & 1 \cdot (-1) & 1 \cdot (-1) & -1 \cdot (-1) \\
E_1 \cdot (B) & 2 \cdot 1 & -1 \cdot 1 & 0 \cdot 1 & 2 \cdot (-1) & -1 \cdot (-1) & 0 \cdot (-1) \\
\end{array}
\]
\[ D_6 \supset D_2 \supset C_2 = D_3 \times C_2 \] Irreducible characters

<table>
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<tr>
<th>( D_3 )</th>
<th>1 ( { r, r^2 } )</th>
<th>( i_1, i_2, i_3 )</th>
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<tr>
<td>( \chi^A(g) )</td>
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<td>1</td>
</tr>
<tr>
<td>( \chi^{A_2}(g) )</td>
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<td>1</td>
</tr>
<tr>
<td>( \chi^E(g) )</td>
<td>2</td>
<td>-1</td>
</tr>
</tbody>
</table>

\[ D_3 \times C_2^Z \begin{array}{ccc|ccc|ccc} \chi^A(g) & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ \chi^{A_2}(g) & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 \\ \chi^E(g) & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ \end{array} \]

\[ D_3 \times C_2^Z \begin{array}{ccc|ccc|ccc} \chi^A(g) & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ \chi^{A_2}(g) & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 \\ \chi^E(g) & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ \end{array} \]

\[ D_3 \times C_2^Z \begin{array}{ccc|ccc|ccc} \chi^A(g) & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ \chi^{A_2}(g) & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 \\ \chi^E(g) & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ \end{array} \]

\[ D_3 \times C_2^Z \begin{array}{ccc|ccc|ccc} \chi^A(g) & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ \chi^{A_2}(g) & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 \\ \chi^E(g) & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ \end{array} \]
$D_6 \supseteq D_2 \supseteq C_2 = D_3 \times C_2$ Irreducible characters

Recall $C_2 \times C_2 = D_2 = \{1, R_x, R_z, R_y\}$ characters

$Lect.12$ p.50-60

$D_6$ has $D_2 = \{1, i_3, h^3, j_3\}$ subgroup
\[ D_6 \supset D_2 \supseteq C_2 = D_3 \times C_2 \] Irreducible characters

Recall \( C_2 \times C_2 = D_2 = \{1, R_x, R_y, R_z\} \) characters

(Lect. 12 p. 50-60)

\( D_6 \) has \( D_2 = \{1, i_3, h^3, j_3\} \) subgroup

\[
\begin{array}{c|ccc|c|ccc}
D_3 & 1 \{r, r^2\} & \{i_1, i_2, i_3\} & C_2^Z & 1 \{r\} & \{i_1, i_2, i_3\} & 1 \cdot R_z & \{r, r^2\} \cdot R_z & \{i_1, i_2, i_3\} \cdot R_z \\
\hline
1 & 1 & 1 & (A) & 1 & 1 & 1 & 1 & 1 \\
D & 1 & 1 & (A) & 1 & 1 & -1 & 1 & -1 \\
D & 1 & 1 & (B) & 1 & -1 & 1 & 0 & -1 \\
D & 1 & 1 & (B) & 1 & -1 & -1 & 1 & -1 \\
D & 1 & 1 & (B) & 2 & -1 & 0 & -1 & 0 \\
\hline
D_3 \times C_2^Z & 1 \{h^2, h^4\} & \{i_1, i_2, i_3\} & h^3 & \{h, h^5\} & \{j_1, j_2, j_3\} & 1 & 1 & 1 & 1 \\
\hline
\hline
A_1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
A_2 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 \\
E_2 & 2 & -1 & 0 & 2 & -1 & 0 & 0 & 0 \\
B_1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\
B_2 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 \\
E_1 & 2 & -1 & 0 & -2 & 1 & 0 & 0 & 0 \\
\hline
\end{array}
\]
$D_6 \supseteq D_2 \supseteq C_2 = D_3 \times C_2$ Irreducible characters

<table>
<thead>
<tr>
<th>$D_3$</th>
<th>1</th>
<th>${r, r^2}$</th>
<th>${i_1, i_2, i_3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi^A(g)$</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$\chi^B(g)$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$\chi^C(g)$</td>
<td>2</td>
<td>-1</td>
<td>0</td>
</tr>
</tbody>
</table>

$C_2^\times C_2 = 1 \{r, r^2\} \{i_1, i_2, i_3\}$ characters

$(Lect.12.p.50-60)$

$D_6$ has $D_2 = \{1, i_3, h^3, j_3\}$ subgroup

$R_z(180^\circ)$

$D_2$

<table>
<thead>
<tr>
<th>$1$</th>
<th>$R_X$</th>
<th>$R_Z$</th>
<th>$R_Y$</th>
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<td>$R_Y$</td>
<td>$R_Z$</td>
<td>$R_X$</td>
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</tr>
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</table>

$D_3 \times C_2^Z$

$X\text{-}rotation$ $\text{or}$ $180^\circ \text{X\text{-}flip i}_3$

$A_1$ or $B_1$ vs $A_2$ or $B_2$

$(+1)$ vs $(-1)$

Let $X\text{-}rotation$ $\text{or}$ $60^\circ \text{hex-Z rotation h}$

$A_p$ vs $B_p$

$(+1)$ vs $(-1)$

So also does: $180^\circ h^3$
Review: Symmetry reduction and splitting: Subduced irep $D^\alpha(D_3)\downarrow C_2 = d^{02} \oplus d^{12} \oplus \ldots$ correlation
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$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry
Irreducible characters
Irreducible representations
Correlations with $D_6$ characters:
...and $C_2(i_3)$ characters......and $C_6(1,h^1,h^2,\ldots)$ characters
$D_6$ symmetry and induced representation band structure

Introduction to octahedral tetrahedral symmetry $O_h \supset O \sim T_d \supset T$
$D_6 \cong D_2 \cong C_2 = D_3 \times C_2$ Irreducible representations

| g = | 1 , | r = h^2 , | r^2 = h^4 , | i_1 | i_2 | i_3 | h^3 | h^3 r = h^5 | h^3 r^2 = h^1 | h^3 i_1 = j_1 | h^3 i_2 = j_2 | h^3 i_3 = j_3 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| $D_{A_1}^I (g)$ | 1 , | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $D_{A_2}^I (g)$ | 1 , | 1 | 1 | -1 | -1 | -1 | 1 | 1 | 1 | -1 | -1 |
| $D_{E_2}^I (g)$ | (1 0) | (1 0) | (1 0) | (1 0) | (1 0) | (1 0) | (1 0) | (1 0) | (1 0) | (1 0) | (1 0) |
| $D_{E_1}^I (g)$ | (0 1) | (0 1) | (0 1) | (0 1) | (0 1) | (0 1) | (0 1) | (0 1) | (0 1) | (0 1) | (0 1) |

Diagrams showing the rotations and symmetries of $D_6$.
\[ D_6 \triangleright D_2 \triangleright C_2 = D_3 \times C_2 \]

Irreducible representations

<table>
<thead>
<tr>
<th>( g )</th>
<th>( 1 )</th>
<th>( r = h^2 )</th>
<th>( r^2 = h^4 )</th>
<th>( i_1 )</th>
<th>( i_2 )</th>
<th>( i_3 )</th>
<th>( h^3 )</th>
<th>( h^3 \mathbf{r} = h^5 )</th>
<th>( h^3 \mathbf{r}^2 = h^1 )</th>
<th>( h^3 i_1 = j_1 )</th>
<th>( h^3 i_2 = j_2 )</th>
<th>( h^3 i_3 = j_3 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D^A_1(g) )</td>
<td>( \begin{pmatrix} 1 &amp; 1 &amp; 1 &amp; 1 &amp; 1 &amp; 1 &amp; 1 &amp; 1 &amp; 1 \end{pmatrix} )</td>
<td></td>
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</tr>
<tr>
<td>( D^A_2(g) )</td>
<td>( \begin{pmatrix} 1 &amp; 1 &amp; 1 &amp; 1 &amp; -1 &amp; -1 &amp; -1 &amp; -1 &amp; -1 \end{pmatrix} )</td>
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<tr>
<td>( D^E_2(g) )</td>
<td>( \begin{pmatrix} 1 &amp; 0 \ 0 &amp; 1 \end{pmatrix} )</td>
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<tr>
<td>( D^B_1(g) )</td>
<td>( \begin{pmatrix} 1 &amp; 1 &amp; 1 &amp; 1 &amp; 1 &amp; 1 &amp; 1 &amp; 1 &amp; 1 \end{pmatrix} )</td>
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</tr>
<tr>
<td>( D^B_2(g) )</td>
<td>( \begin{pmatrix} 1 &amp; 1 &amp; 1 &amp; 1 &amp; -1 &amp; -1 &amp; -1 &amp; -1 &amp; -1 \end{pmatrix} )</td>
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<tr>
<td>( D^E_1(g) )</td>
<td>( \begin{pmatrix} 1 &amp; 0 \ 0 &amp; 1 \end{pmatrix} )</td>
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</tbody>
</table>

Let \( X \)-rotation or \( 180^\circ \) \textbf{X-flip} \( i_3 \)
determines

\[ A_1 \text{ or } B_1 \text{ vs } A_2 \text{ or } B_2 \]

\( (+1) \text{ vs } (-1) \)
Irreducible representations

\[ D_6 \cong D_2 \cong C_2 = D_3 \times C_2 \]

Let \( \mathbf{X} \)-rotation or \( \mathbf{Z} \)-rotation determine:

- \( A_1 \) or \( B_1 \) vs \( A_2 \) or \( B_2 \)
- \( +1 \) vs \(-1\)

Let unit translation or 60° hex-\( \mathbf{Z} \) rotation determine:

- \( A_p \) vs \( B_p \)
- \( +1 \) vs \(-1\)

So also does: 180° \( \mathbf{h}^3 \)
$D_6 \triangleleft D_2 \triangleleft C_2 = D_3 \times C_2$ Irreducible representations

Let $X$-rotation or $180^\circ$ X-flip $i_3$ determine $A_1$ or $B_1$ vs $A_2$ or $B_2$ (+1) vs (-1)

Let unit translation or $60^\circ$ hex-$Z$ rotation $h$ determine $A_p$ vs $B_p$ (+1) vs (-1)

So also does: $180^\circ h^3$

Y-rotation or $180^\circ$ flip $j_3$ is product $i_3 h^3 = h^3 i_3$
Review: Symmetry reduction and splitting: Subduced irep $D^\alpha(D_3) \downarrow C_2 = d^{02} \oplus d^{12} \oplus \ldots$ correlation
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$D_6$ symmetry and induced representation band structure

Introduction to octahedral tetrahedral symmetry $O_h \supset O \sim T_d \supset T$
Correlations by $D_6$ characters: $\chi^\mu_g(D_6) =$

\[
\begin{array}{c|cccc|ccc}
D_3 \times C^\infty_2 & 1 & \{h^2, h^4\} & \{i_1, i_2, i_3\} & h^3 & \{h, h^5\} & \{j_1, j_2, j_3\} \\
\hline
A_1 & 1 & 1 & 1 & 1 & 1 & 1 \\
A_2 & 1 & 1 & -1 & 1 & 1 & -1 \\
E_2 & 2 & -1 & 0 & 2 & -1 & 0 \\
B_1 & 1 & 1 & 1 & -1 & -1 & -1 \\
B_2 & 1 & 1 & -1 & -1 & -1 & 1 \\
E_1 & 2 & -1 & 0 & -2 & 1 & 0 \\
\end{array}
\]

...and $C_2(i_3)$ characters:

\[
\begin{array}{c|cc|c}
C^X_2 & 1 & i_3 & \\
\hline
0_2 & 1 & 1 & \\
l_2 & 1 & -1 & \\
\end{array}
\]

Let $X$-rotation or $180^\circ X$-flip $i_3$ determine $A_1$ or $B_1$ vs $A_2$ or $B_2$ (+1) vs (-1)

\[
\begin{array}{c|cc|c}
D_6 \supseteq C^X_2(i_3) & 0_2 & l_2 \\
\hline
A_1 & 1 & . \\
A_2 & . & 1 \\
E_2 & 1 & 1 \\
B_1 & 1 & . \\
B_2 & . & 1 \\
E_1 & 1 & 1 \\
\end{array}
\]
Correlations by $D_6$ characters: $\chi^\mu_g(D_6) =$

...and $C_2(i_3)$ characters:

\[
\begin{array}{c|cc}
C_2^X & 1 & i_3 \\
\hline
0_2 & 1 & 1 \\
1_2 & 1 & -1 \\
\end{array}
\]

...and $C_6(1,h^1,h^2,...)$ characters:

Let $X$-rotation or $180^\circ$ $X$-flip $i_3$ determine $A_1$ or $B_1$ vs $A_2$ or $B_2$ (+1) vs (-1)

Let unit translation or $60^\circ$ hex-$Z$ rotation $h$ determine $A_p$ vs $B_p$ (+1) vs (-1)

So also does: $180^\circ h^3$

\[
\begin{array}{c|c|c|c|c|c|c}
D_3 \times C_2^z & 1 & \{h^2,h^4\} & \{i_1,i_2,i_3\} & h^3 & \{h,h^5\} & \{j_1,j_2,j_3\} \\
\hline
A_1 & 1 & 1 & 1 & 1 & 1 & 1 \\
A_2 & 1 & 1 & -1 & 1 & 1 & -1 \\
E_2 & 2 & -1 & 0 & 2 & -1 & 0 \\
\hline
B_1 & 1 & 1 & 1 & -1 & -1 & -1 \\
B_2 & 1 & 1 & -1 & -1 & -1 & 1 \\
E_1 & 2 & -1 & 0 & -2 & 1 & 0 \\
\end{array}
\]

$(\varepsilon = e^{\pi i/3})$

\[\varepsilon=\frac{e^{\pi i/3}}{3}\]
Correlations by $D_6$ characters: $\chi^\mu(D_6) =$

<table>
<thead>
<tr>
<th>$D_3 \times C_2^Z$</th>
<th>$1 {h^2,h^4}$</th>
<th>${i_1,i_2,i_3}$</th>
<th>$h^3$</th>
<th>${h,h^5}$</th>
<th>${j_1,j_2,j_3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1 1</td>
<td>1</td>
<td>1</td>
<td>1 1</td>
<td>1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1 1</td>
<td>-1</td>
<td>1</td>
<td>1 -1</td>
<td>0</td>
</tr>
<tr>
<td>$E_2$</td>
<td>2 -1</td>
<td>0</td>
<td>2</td>
<td>-1</td>
<td>0</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1 1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_2$</td>
<td>1 1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$E_1$</td>
<td>2 -1</td>
<td>0</td>
<td>-2</td>
<td>1</td>
<td>0</td>
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</table>

...and $C_2(i_3)$ characters:

<table>
<thead>
<tr>
<th>$C_2^X$</th>
<th>$i_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
</tr>
</tbody>
</table>

...and $C_6(1,h^1,h^2,...)$ characters:

Let $X$-rotation or

180° $X$-flip $i_3$

determine $A_1$ or $B_1$ vs $A_2$ or $B_2$

(1) $vs$ (-1)

**So also does:** 180° $h^3$

Let unit translation or

60° hex-$Z$ rotation $h$

determine $A_p$ vs $B_p$

(+1) vs (-1)

180° flip $j_3$

is product $i_3h^3 = h^3i_3$

$D_6 \supset C_2^X(i_3)$

<table>
<thead>
<tr>
<th>$D_6 \supset C_6(h)$</th>
<th>$0_6$</th>
<th>$1_6$</th>
<th>$2_6$</th>
<th>$3_6$</th>
<th>$4_6$</th>
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<tbody>
<tr>
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</table>

$\varepsilon = e^{2\pi/3}$
Review: Symmetry reduction and splitting: Subduced irep \( D^\alpha(D_3) \downarrow C_2 = d^{02} \oplus d^{12} \oplus \ldots \) correlation
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\( D_6 \rhd D_2 \rhd C_2 = D_3 \times C_2 \) symmetry and outer product geometry
- Irreducible characters
- Irreducible representations
- Correlations with \( D_6 \) characters:
  ...and \( C_2(i_3) \) characters......and \( C_6(1,h^1,h^2,...) \) characters
- \( D_6 \) symmetry and induced representation band structure

Introduction to octahedral tetrahedral symmetry\( O_h \supset O \sim T_d \supset T \)
For low energy deep in potential local $C_2$ symmetry dominates and the bands $A_1E_1E_2B_1$ and $B_2E_2E_1A_2$ that become tight clusters

<table>
<thead>
<tr>
<th>$D_3 \supset C_2(j_3)$</th>
<th>0_2</th>
<th>1_2</th>
</tr>
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<tbody>
<tr>
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<td>$B_2$</td>
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<tr>
<td>$B_1$</td>
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<td>.</td>
</tr>
<tr>
<td>$E_1$</td>
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</tbody>
</table>

For high energy above potential barriers local $C_2$ symmetry is replaced by global $C_6$ angular momentum doublets such as $E_{\pm m}, A_1A_2,$ and $B_1B_2$
For low energy deep in potential local $C_2$ symmetry dominates and the bands $A_1E_1E_2B_1$ and $B_2E_2E_1A_2$ then become tight clusters.

For high energy above potential barriers local $C_2$ symmetry is replaced by global $C_6$ angular momentum doublets such as $E_\pm m$, $A_1A_2$, and $B_1B_2$.

$$D_6 \supset C_3(h)$$

<table>
<thead>
<tr>
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<th>$2_6$</th>
<th>$3_6$</th>
<th>$4_6$</th>
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<td>$E_2$</td>
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<td>1</td>
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<tr>
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$$D_6 \supset C_2(j_3)$$

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<tr>
<td>$B_2$</td>
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<tr>
<td>$B_1$</td>
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<td>.</td>
</tr>
<tr>
<td>$E_1$</td>
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</table>
Symmetry reduction and splitting: Subduced rep $D^\alpha(D_3)\downarrow C_2 = d_0^2 \oplus d_1^2 \oplus \ldots$ correlation

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$D_3$-Projection of $d^{m_2}(C_2)\uparrow D_3$ induced representation basis

Derivation of Frobenius reciprocity

$D_6 \supset D_2 \supset C_2 = D_3 \times C_2$ symmetry and outer product geometry

Irreducible characters

Irreducible representations

Correlations with $D_6$ characters:

...and $C_2(i_3)$ characters......and $C_6(1,h^1,h^2,...)$ characters

$D_6$ symmetry and induced representation band structure

Introduction to octahedral/tetrahedral symmetry $O_h \supset O \sim T_d \supset T$
$O_h \supset O \supset D_4 \supset C_{4v} \supset C_{2v}$ subgroup chain

...(one of very many)
$O_h \supset O \supset D_4 \supset C_4$ subgroup chain

...(one of my favorites)
Three groups: $O$, $D_4$, and $D_3$ let you “do” all the other 32 crystal point groups.
Introduction to octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

Octahedral-cubic $O$ symmetry

Order $^pO = 6$ hexahedron squares · 4 pts $= 24$
$= 8$ octahedron triangles · 3 pts $= 24$
$= 12$ lines · 2 pts $= 24$ positions
Introduction to octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

Octahedral-cubic $O$ symmetry

Order $^O = 6$ hexahedron squares $\cdot 4$ pts $= 24$
$= 8$ octahedron triangles $\cdot 3$ pts $= 24$
$= 12$ lines $\cdot 2$ pts $= 24$ positions

Octahedral group $O$ operations

Class of 1: $1$

Class of 6: $\pm 90^\circ$ rotations on $[100]$ axes

Class of 3: $180^\circ$ rotations on $[100]$ axes

Class of 8: $120^\circ$ rotations on $[111]$ axes

Tuesday, March 31, 2015
Introduction to octahedral/tetrahedral symmetry $O_h \supseteq O \sim T_d \supseteq T$

Octahedral-cubic $O$ symmetry

Order $\circ O = 6$ hexahedron squares $\cdot$ 4 pts $= 24$
$= 8$ octahedron triangles $\cdot$ 3 pts $= 24$
$= 12$ lines $\cdot$ 2 pts $= 24$ positions

Eight classes of symmetry:

1. Class of 1: $1$
   - $r_k = r_k$

2. Class of 8: $120^\circ$ rotations on [111] axes

3. Class of 6 $\pm 90^\circ$ rotations on [100] axes

4. Class of 3 $180^\circ$ rotations on [100] axes
Introduction to octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

**Octahedral-cubic O symmetry**

Order $\circ O = 6$ hexahedron squares $\cdot$ $4$ pts $= 24$

$= 8$ octahedron triangles $\cdot$ $3$ pts $= 24$

$= 12$ lines $\cdot$ $2$ pts $= 24$ positions

**Octahedral group O operations**

Class of 1: $\mathbf{1}$

$r_k = r_k$

Class of 8: $120^\circ$ rotations on $[111]$ axes

$\rho_{x,y,z} = R_{1,2,3}^2$

Class of 3 $180^\circ$ rotations on $[100]$ axes

Class of 2: $r_k^2 = r_k^{-1}$
Introduction to octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

Octahedral-cubic $O$ symmetry

Order $^\circ O = 6$ hexahedron squares $\cdot$ 4 pts $= 24$
$= 8$ octahedron triangles $\cdot$ 3 pts $= 24$
$= 12$ lines $\cdot$ 2 pts $= 24$ positions

Octahedral group $O$ operations

Class of 1: 1
$r_k = r_k$

Class of 8: 120° rotations on [111] axes
$R_{x,y,z} = R_{1,2,3}$

Class of 3 180° rotations on [100] axes
$\rho_{x,y,z} = R_{1,2,3}^2$

Class of 6 $\pm 90°$ rotations on [100] axes
$R_{x,y,z} = R_{1,2,3} = R_{1,2,3}^{-1}$
Introduction to octahedral/tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

Octahedral-cubic $O$ symmetry

Order $O = 6$ hexahedron squares · 4 pts = 24
$= 8$ octahedron triangles · 3 pts = 24
$= 12$ lines · 2 pts = 24 positions

Octahedral group $O$ operations

Class of 1: $1$
$r_k = r_k$

Class of 8: 120° rotations on [111] axes

Class of 6: ±90° rotations on [100] axes

Class of 3: 180° rotations on [100] axes

Class of 8: 120° rotations on [111] axes

Class of 1: $1$

$\rho_{x,y,z} = R_{1,2,3}$
$\tilde{R}_{x,y,z} = R_{1,2,3}$

$R_{x,y,z} = R_{1,2,3}$

$\tilde{R}_{x,y,z} = R_{1,2,3}^{-1}$

$\tilde{R}_{x,y,z} = R_{1,2,3}$
Introduction to octahedral/ tetrahedral symmetry \(O_h \supset O \sim T_d \supset T\)

**Octahedral-cubic O symmetry**

**Octahedral group O operations**

Class of 1: \(1\)
\[ r_k = r_k \]

Class of 8:
\(\pm 120^\circ\) rotations on [111] axes
\[ r_k^2 = r_k^{-1} \]
\[ \rho_{x,y,z} = R_{1,2,3} \]

Class of 6:
\(\pm 90^\circ\) rotations on [100] axes
\[ R_{x,y,z} = R_{1,2,3} \]

Class of 3:
180\(^\circ\) rotations on [100] axes
\[ \rho_{x,y,z} = R_{1,2,3} \]

Class of 8:
\(\pm 120^\circ\) rotations on [111] axes
\[ \rho_{x,y,z} = R_{1,2,3} \]

Class of 6:
180\(^\circ\) rotations on [110] diagonals
\[ \rho_i = i_k \]

Order \(\circ O = 6\) hexahedron squares \(\cdot 4\) pts = 24
= 8 octahedron triangles \(\cdot 3\) pts = 24
= 12 lines \(\cdot 2\) pts = 24 positions
Introduction to octahedral/ tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

**Octahedral-cubic O symmetry**

Octahedral group $O$ operations

- **Class of 1:** $1$
  - $r_k = r_k$

- **Class of 8:** $\pm 120^\circ$ rotations on [111] axes
  - $R_{x,y,z} = R_{1,2,3}$

- **Class of 6:** $\pm 90^\circ$ rotations on [100] axes
  - $\rho_{x,y,z} = R_{1,2,3}^2$

- **Class of 6:** $180^\circ$ rotations on [100] axes

- **Class of 3:** $180^\circ$ rotations on [110] diagonals
  - $i_k = i_k$

- **Class of 8:** $\pm 120^\circ$ rotations on [111] axes

**Tetrahedral symmetry becomes Icosahedral**

Order $\circ O = 6$ hexahedron squares $\cdot 4$ pts $= 24$

$= 8$ octahedron triangles $\cdot 3$ pts $= 24$

$= 12$ lines $\cdot 2$ pts $= 24$ positions

(If rectangles have Golden Ratio $1 + \sqrt{5}/2$)

---

Tuesday, March 31, 2015
Introduction to octahedral tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

Octahedral groups $O_h \supset O \sim T_d \supset T$

Figure 4.1.5 The full octahedral group ($O_h$) and four non-Abelian subgroups $T$, $T_h$, $T_d$, and $O$. The Abelian $D_2$ subgroup of $T$ is indicated also.
Introduction to octahedral tetrahedral symmetry $O_h \supset O \sim T_d \supset T$

Octahedral groups $O_h \supset O \sim T_d \supset T$

*Figure 4.1.5* The full octahedral group ($O_h$) and four non-Abelian subgroups $T$, $T_h$, $T_d$, and $O$. The Abelian $D_2$ subgroup of $T$ is indicated also.
Introduction to octahedral tetrahedral symmetry \( O_h \supset O \sim T_d \supset T \)

Octahedral groups \( O_h \supset O \sim T_d \) and \( O_h \supset T_h \supset T \)

**Figure 4.1.5** The full octahedral group \( (O_h) \) and four non-Abelian subgroups \( T, T_h, T_d, \) and \( O \). The Abelian \( D_2 \) subgroup of \( T \) is indicated also.

*Fig. 4.1.5 from Principles of Symmetry, Dynamics and Spectroscopy*
Octahedral rotation product Table F.2.1 from Principles of Symmetry, Dynamics and Spectroscopy

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Note: The table represents the octahedral rotation product and is derived from the principles of symmetry, dynamics, and spectroscopy.
Example: $G=O$ Centrum: $\kappa(O) = \sum_{\alpha} (\ell^\alpha)^0 = 1^0 + 1^0 + 2^0 + 3^0 + 3^0 = 5$

Cubic-Octahedral Group $O$

Rank: $\rho(O) = \sum_{\alpha} (\ell^\alpha)^l = 1^1 + 1^1 + 2^1 + 3^1 + 3^1 = 10$

Order: $^0(O) = \sum_{\alpha} (\ell^\alpha)^0 = 1^2 + 1^2 + 2^2 + 3^2 + 3^2 = 24$

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$O \supset C_4$

$O \supset C_3$

$\mathcal{O} \supset C_4$

$\mathcal{O} \supset C_3$

$\rho = (0)_4 (1)_4 (2)_4 (3)_4 = (-1)_4$

$\rho = (0)_3 (1)_3 (2)_3 = (-1)_3$
Primary AET species mixing increases with distance from "separatrix".

Observed repeating sequence(s)...

Local correlations explain clustering...
... but what about spacing and ordering?...
...and physical consequences?
Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = g |I\rangle$ of position ket $|g\rangle$