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2 Exercise - Introduction to Group Theory

2.1 (groups from adding or deleting a symmetry operation)

C_3 plus i leads to S_6	S_6 minus i leads to C_3	D_{3d} minus S_6 leads to D_3
C_{3v} plus i leads to D_{3h}	T_d plus i leads to O_h	S_4 plus i leads to C_{4h}
C_{5v} plus σ_h leads to D_{5h}	C_3 plus S_6 leads to S_6	C_{3h} minus ${S_6}^5$ leads to C_{3h}

Looking at C_{3h} we don't find ${S_6}^5$, that's why it won't change the point group to subtract it. If we were meant to subtract ${S_3}^5$ we get the point group C_3.

2.2 (Decomposition of the reducible representations of D_4)

D_4	E	$2C_4$	C_2	$2C_2'$	$2C_2''$
Γ_1	3	-1	-1	1	-1
Γ_2	2	2	2	0	0
Γ_3	8	0	0	0	0
Γ_4	4	-2	0	-2	2

We first have to check if the representations are reducible, therefore we check the condition for irreducible representations:

$$\sum_R \chi\left[\Gamma_i(R)\right]^* \chi\left[\Gamma_j(R)\right] = h\delta_{ij}$$

with $i = j$ this leads to the condition:

$$\sum_i l_i^2 = h$$

with l_i being the dimension of the i-th irreducible representation of a group of order h. Using the character table of D_4:

D_4	E	$2C_4$	C_2	$2C_2'$	$2C_2''$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	-1	1	1	-1
B_2	1	-1	1	-1	1
E	2	0	-2	0	0

we find the order of h:

$$\sum_i l_i^2 = 1^2 + 1^2 + 1^2 + 1^2 + 2^2 = 8 = h$$

Therefore the representation will be reducible if $\sum_i l_i^2 = 8$.

$$
\begin{array}{lll}
\Gamma_1: & 1\cdot|3|^2+2\cdot|-1|^2+1\cdot|-1|^2+2\cdot|1|^2+2\cdot|-1|^2=16>8, & \text{reducible}\\
\Gamma_2: & 1\cdot|2|^2+2\cdot|2|^2+1\cdot|2|^2+2\cdot|0|^2+2\cdot|0|^2=16>8, & \text{reducible}\\
\Gamma_3: & 1\cdot|8|^2+2\cdot|2|^2+1\cdot|0|^2+2\cdot|0|^2+2\cdot|0|^2=72>8, & \text{reducible}\\
\Gamma_4: & 1\cdot|4|^2+2\cdot|-2|^2+1\cdot|0|^2+2\cdot|-2|^2+2\cdot|2|^2=40>8, & \text{reducible}
\end{array}
$$

We can now decompose the reducible representations using the formula:

$$m_i=\frac{1}{h}\sum_i c_i\chi\left[\Gamma_i\left(R\right)\right]^*\chi\left[\Gamma_i\left(R\right)\right]$$

where m_i stands for the irreducible representations ($m_1=A_1$, $m_2=A_2$, $m_3=B_1$, $m_4=B_2$, $m_5=E$). We now decompose, starting from Γ_1:

$$
\begin{aligned}
A_1 &= \frac{1}{8}\left[1\cdot1\cdot3+2\cdot1\cdot(-1)+1\cdot1\cdot(-1)+2\cdot1\cdot1+2\cdot1\cdot(-1)\right]=\frac{1}{8}\left(3-2-1+2-2\right)=0\\
A_2 &= \frac{1}{8}\left[1\cdot1\cdot3+2\cdot1\cdot(-1)+1\cdot1\cdot(-1)+2\cdot(-1)\cdot1+2\cdot(-1)\cdot(-1)\right]=\frac{1}{8}\left(3-2-1-2+2\right)=0\\
B_1 &= \frac{1}{8}\left[1\cdot1\cdot3+2\cdot(-1)\cdot(-1)+1\cdot1\cdot(-1)+2\cdot1\cdot1+2\cdot(-1)\cdot(-1)\right]=\frac{1}{8}\left(3+2-1+2+2\right)=1\\
B_2 &= \frac{1}{8}\left[1\cdot1\cdot3+2\cdot(-1)\cdot(-1)+1\cdot1\cdot(-1)+2\cdot(-1)\cdot1+2\cdot1\cdot(-1)\right]=\frac{1}{8}\left(3+2-1-2-2\right)=0\\
E &= \frac{1}{8}\left[1\cdot2\cdot3+2\cdot0\cdot(-1)+1\cdot(-2)\cdot(-1)+2\cdot0\cdot1+2\cdot0\cdot(-1)\right]=\frac{1}{8}\left(6+2\right)=1
\end{aligned}
$$

now Γ_2:

$$
\begin{aligned}
A_1 &= \frac{1}{8}\left[1\cdot1\cdot2+2\cdot1\cdot2+1\cdot1\cdot2+2\cdot1\cdot0+2\cdot1\cdot0\right]=\frac{1}{8}\left(2+4+2+0+0\right)=1\\
A_2 &= \frac{1}{8}\left[1\cdot1\cdot2+2\cdot1\cdot2+1\cdot1\cdot2+2\cdot(-1)\cdot0+2\cdot(-1)\cdot0\right]=\frac{1}{8}\left(2+4+2+0+0\right)=1\\
B_1 &= \frac{1}{8}\left[1\cdot1\cdot2+2\cdot(-1)\cdot2+1\cdot1\cdot2+2\cdot1\cdot0+2\cdot(-1)\cdot0\right]=\frac{1}{8}\left(2-4+2+0+0\right)=0\\
B_2 &= \frac{1}{8}\left[1\cdot1\cdot2+2\cdot(-1)\cdot2+1\cdot1\cdot2+2\cdot(-1)\cdot0+2\cdot1\cdot0\right]=\frac{1}{8}\left(2-4+2+0+0\right)=0\\
E &= \frac{1}{8}\left[1\cdot2\cdot2+2\cdot0\cdot2+1\cdot(-2)\cdot2+2\cdot0\cdot0+2\cdot0\cdot0\right]=\frac{1}{8}\left(4+0-4+0+0\right)=0
\end{aligned}
$$

for Γ_3:

$$
\begin{aligned}
A_1 &= \frac{1}{8}\left[1\cdot1\cdot8+2\cdot1\cdot0+1\cdot1\cdot0+2\cdot1\cdot0+2\cdot1\cdot0\right]=\frac{1}{8}\left(8+0+0+0+0\right)=1\\
A_2 &= \frac{1}{8}\left[1\cdot1\cdot8+2\cdot1\cdot0+1\cdot1\cdot0+2\cdot(-1)\cdot0+2\cdot(-1)\cdot0\right]=\frac{1}{8}\left(8+0+0+0+0\right)=1\\
B_1 &= \frac{1}{8}\left[1\cdot1\cdot8+2\cdot(-1)\cdot0+1\cdot1\cdot0+2\cdot1\cdot0+2\cdot(-1)\cdot0\right]=\frac{1}{8}\left(8+0+0+0+0\right)=1\\
B_2 &= \frac{1}{8}\left[1\cdot1\cdot8+2\cdot(-1)\cdot0+1\cdot1\cdot0+2\cdot(-1)\cdot0+2\cdot1\cdot0\right]=\frac{1}{8}\left(8+0+0+0+0\right)=1\\
E &= \frac{1}{8}\left[1\cdot2\cdot8+2\cdot0\cdot0+1\cdot(-2)\cdot0+2\cdot0\cdot0+2\cdot0\cdot0\right]=\frac{1}{8}\left(16+0+0+0+0\right)=2
\end{aligned}
$$

and finally Γ_4:

$$
\begin{aligned}
A_1 &= \frac{1}{8}\left[1\cdot 1\cdot 4 + 2\cdot 1\cdot(-2) + 1\cdot 1\cdot 0 + 2\cdot 1\cdot(-2) + 2\cdot 1\cdot 2\right] = \frac{1}{8}\left(4-4+0-4+4\right) = 0 \\
A_2 &= \frac{1}{8}\left[1\cdot 1\cdot 4 + 2\cdot 1\cdot(-2) + 1\cdot 1\cdot 0 + 2\cdot(-1)\cdot(-2) + 2\cdot(-1)\cdot 2\right] = \frac{1}{8}\left(4-4+0+4-4\right) = 0 \\
B_1 &= \frac{1}{8}\left[1\cdot 1\cdot 4 + 2\cdot(-1)\cdot(-2) + 1\cdot 1\cdot 0 + 2\cdot 1\cdot(-2) + 2\cdot(-1)\cdot 2\right] = \frac{1}{8}\left(4+4+0-4-4\right) = 0 \\
B_2 &= \frac{1}{8}\left[1\cdot 1\cdot 4 + 2\cdot(-1)\cdot(-2) + 1\cdot 1\cdot 0 + 2\cdot(-1)\cdot(-2) + 2\cdot 1\cdot 2\right] = \frac{1}{8}\left(4+4+0+4+4\right) = 2 \\
E &= \frac{1}{8}\left[1\cdot 2\cdot 4 + 2\cdot 0\cdot(-2) + 1\cdot(-2)\cdot 0 + 2\cdot 0\cdot(-2) + 2\cdot 0\cdot 2\right] = \frac{1}{8}\left(8+0+0+0+0\right) = 1
\end{aligned}
$$

We can write this in short form:

$$
\begin{aligned}
\Gamma_1 &= B_1 + E \\
\Gamma_2 &= A_1 + A_2 \\
\Gamma_3 &= A_1 + A_2 + B_1 + B_2 + 2\cdot E \\
\Gamma_4 &= 2\cdot B_1 + E
\end{aligned}
$$

This finally can be written in a nice matrixform of:

	Γ_1	Γ_2	Γ_3	Γ_4
A_1	0	1	1	0
A_2	0	1	1	0
B_1	1	0	1	0
B_2	0	0	1	2
E	1	0	2	1

2.3 (Point groups of substituted cyclobutanes)

a. C_S

b. C_{2v}

c. C_S

d. C_2

e. C_{2v}

f. C_{2h}

g. C_S

h. C_{4v}

i. D_{2h}

k. C_{2h}

l. D_{2d}

m. S_2