Symmetry and Group Theory – Exercise Set 4, Solutions

4.1) Determine the classes of symmetry operations in C_{3v}.

$C_{3v} = \{E, C_3, C_3^2, \sigma_v, \sigma_v', \sigma_v''\}$, $h = 6$

Since E commutes with every other element, it forms a class of its own.

Since C_3 and C_3^2 commute, their similarity transforms do not tell us anything new.

$$(C_3^2)^{-1} C_3 C_3^2 = C_3$$
$$C_3^{-1} C_3^2 C_3 = C_3^2$$

We have more luck by transforming a rotation with a reflection.

Solution using conventions from Ulrich Lorenz's lecture notes:

$$\sigma_v^{xz} C_3 \sigma_v^{xz} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\frac{2\pi}{3} & \sin\frac{2\pi}{3} & 0 \\ -\sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos\frac{2\pi}{3} & -\sin\frac{2\pi}{3} & 0 \\ \sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$= C_3^2$$

Therefore, C_3 and C_3^2 are conjugate.

If we transform a reflection with a rotation, we obtain the following.

$$C_3^{-1} \sigma_v^{xz} C_3 = \begin{pmatrix} \cos\frac{2\pi}{3} & -\sin\frac{2\pi}{3} & 0 \\ \sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\frac{2\pi}{3} & \sin\frac{2\pi}{3} & 0 \\ -\sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} \cos\frac{2\pi}{3} & -\sin\frac{2\pi}{3} & 0 \\ \sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\frac{2\pi}{3} & \sin\frac{2\pi}{3} & 0 \\ \sin\frac{2\pi}{3} & -\cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} c^2 - s^2 & 2cs & 0 \\ 2cs & s^2 - c^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \sigma_v'$$

Upon close inspection of the result, we find that $C_3^{-1} \sigma_v^{xz} C_3 = \sigma_v'$, where σ_v' is the second symmetry plane, which is rotated counterclockwise by $\frac{2\pi}{3}$ with respect to σ_v^{xz}. This can be easily verified by a geometrical construction, similar to the one in exercise 1.3 that we used to prove the formula for the rotation matrices.

We could have predicted this result, since the expression $C_3^{-1} \sigma_v^{xz} C_3$ simply represents a coordinate transformation of σ_v^{xz}, in which σ_v^{xz} is rotated counterclockwise by $\frac{2\pi}{3}$. It is therefore clear that

$$(C_3^2)^{-1} \sigma_v^{xz} C_3^2 = \sigma_v''$$

i.e. we obtain the third symmetry plane σ_v'', which is rotated clockwise by $\frac{2\pi}{3}$ with respect to σ_v^{xz}.

Solution using conventions from Jiří Vaníček's lecture and handout:

$$\sigma_v^{yz} C_3 \sigma_v^{yz} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\frac{2\pi}{3} & -\sin\frac{2\pi}{3} & 0 \\ \sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos\frac{2\pi}{3} & \sin\frac{2\pi}{3} & 0 \\ -\sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$= C_3^2$$

Therefore, C_3 and C_3^2 are conjugate.

If we transform a reflection with a rotation, we obtain the following.

$$C_3^{-1} \sigma_v^{yz} C_3 = \begin{pmatrix} \cos\frac{2\pi}{3} & \sin\frac{2\pi}{3} & 0 \\ -\sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\frac{2\pi}{3} & -\sin\frac{2\pi}{3} & 0 \\ \sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} \cos\frac{2\pi}{3} & \sin\frac{2\pi}{3} & 0 \\ -\sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -\cos\frac{2\pi}{3} & \sin\frac{2\pi}{3} & 0 \\ \sin\frac{2\pi}{3} & \cos\frac{2\pi}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} -c^2 + s^2 & 2cs & 0 \\ 2cs & -s^2 + c^2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \sigma_v'$$

Upon close inspection of the result, we find that $C_3^{-1} \sigma_v^{yz} C_3 = \sigma_v'$, where σ_v' is the second symmetry plane, which is rotated counterclockwise by $\frac{4\pi}{3}$ with respect to σ_v^{yz}. This can be easily verified by a geometrical construction, similar to the one in exercise 1.3 that we used to prove the formula for the rotation matrices.

We could have predicted this result, since the expression $C_3^{-1} \sigma_v^{yz} C_3$ simply represents a coordinate transformation of σ_v^{yz}, in which σ_v^{yz} is rotated counterclockwise by $\frac{4\pi}{3}$. It is therefore clear that

$$(C_3^2)^{-1} \sigma_v^{yz} C_3^2 = \sigma_v''$$

i.e. we obtain the third symmetry plane σ_v'', which is rotated counterclockwise by $\frac{2\pi}{3}$ with respect to σ_v^{yz}.

We conclude that the three σ_v planes are all conjugate to each other. Moreover, since the order of a class has to be a divisor of the order of the group, the two conjugate C_3 rotations and the three conjugate σ_v planes cannot belong to the same class. Otherwise, the order of this class would be 5. Instead, we conclude that C_{3v} has the following three classes.

$$\{E\};\ \{C_3, C_3^2\};\ \{\sigma_v, \sigma_v', \sigma_v''\}$$

4.2) Show that by carrying out a similarity transform of one representation of a group $\boldsymbol{G} = \{\boldsymbol{E}, \boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}, \dots\}$, one obtains an isomorphic representation $\boldsymbol{G}' = \{\boldsymbol{E}', \boldsymbol{A}', \boldsymbol{B}', \boldsymbol{C}', \dots\}$.

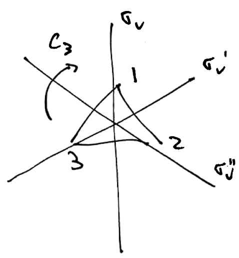
For every product $AB = C$ in the representation G, we can form a product $A'B' = C'$ in the new representation G'

$$A'B' = X^{-1}AX\,X^{-1}BX = X^{-1}ABX = X^{-1}CX = C'$$

which demonstrates that both representations are isomorphic. (Note that the employed "similarity" matrix X is the same for all matrices $E, A, B, C, \dots$ in the original representation.)

4.3) Find a three-dimensional representation of the group C_{3v} by considering the corners of an equilateral triangle as a vector $\boldsymbol{r} = \begin{pmatrix} \mathbf{1} \\ \mathbf{2} \\ \mathbf{3} \end{pmatrix}$.

Solution using conventions from Ulrich Lorenz's lecture notes:
By considering how the different symmetry operations interchange the corners of the triangle, we arrive at the following representation of C_{3v}.

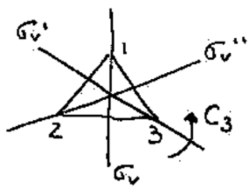


$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, C_3 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, C_3^2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix},$$

$$\sigma_v = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \sigma_v{}' = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \sigma_v{}'' = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

Solution using conventions from Jiří Vaníček's lecture and handout:

We have the following representation:



$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, C_3 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, C_3^2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix},$$

$$\sigma_v = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \sigma_v{}' = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \sigma_v{}'' = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

4.4) Reduce the following reducible representation Γ of C_{3v}.

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0
Γ	6	3	-2

$h = 6$

$$a_1 = \frac{1}{6}(1 \cdot 1 \cdot 6 + 2 \cdot 1 \cdot 3 - 3 \cdot 1 \cdot 2) = 1$$
$$a_2 = \frac{1}{6}(1 \cdot 1 \cdot 6 + 2 \cdot 1 \cdot 3 - 3 \cdot (-1) \cdot 2) = 3$$
$$a_3 = \frac{1}{6}(1 \cdot 2 \cdot 6 + 2 \cdot (-1) \cdot 3 - 3 \cdot 0 \cdot 2) = 1$$

Homework

4.5) Determine the point groups of the following molecules and objects. Which of these molecules and objects can have a permanent dipole moment and which are chiral?

A	C_s
B	C_2
C	D_{3h}
D	$D_{\infty h}$
E	C_{4v}
F	C_3
G	O_h
H	T_d

Permanent dipole moment: A, B, E, F
Chiral: B, F

4.6) If the order of a group is h, can that group have a class that also has order h?

If the group is $\{E\}$, then yes, this obviously is the case.

If the order of the group is larger than 1, $h > 1$, then the identity E always forms a class by itself, since $X^{-1}EX = E$. Therefore, the number of elements of any other class must be smaller than h.

4.7) Show that in an Abelian group of order h, all irreducible representations are one dimensional.

In an Abelian group, all elements are conjugate only to themselves since $X^{-1}AX = X^{-1}XA = A$. Therefore, the group has h classes and therefore also h irreducible representations (Rule 5).

4.8) Complete the character table of D_3. Hint: Use the "Five important rules" for character tables that we have derived using the great orthogonality theorem. Explain how you arrive at the solution. Finding the correct labels for the irreducible representations is not required.

D_3	E	$2C_3$	$3C_2$

Every group has a totally symmetric representation:

D_3	E	$2C_3$	$3C_2$
A_1	1	1	1

Since the number of classes must be equal to the number of irreducible representations (Rule 5), we know that there are two more representations. In other words, the character table is square.

Moreover, since the sum of the squares of the dimensions of all representations must be equal to the order of the group (Rule 1), we can conclude that one of the remaining representations must be one-dimensional, the other one two-dimensional ($1^2 + 1^2 + 2^2 = 6$ is the only solution). Then, we use the fact that the character of E is equal to the dimension of the representation:

D_3	E	$2C_3$	$3C_2$
A_1	1	1	1
A_2	1		
E	2		

We can fill in the rest of the table by recalling that the rows must be orthogonal to each other (Rule 3) and that each row itself must be normalized to the group order (Rule 2). Alternatively, we can use the orthogonality of columns of the character table, which says that $\sum_i \chi_i(R)^* \chi_i(S) = 0$ if R and S belong to different conjugacy classes and $\sum_i \chi_i(R)^* \chi_i(R) = h/n_{c(R)}$, where the sums go over the irreps and $n_{c(R)}$ is the number of elements of the conjugacy class of R:

D_3	E	$2C_3$	$3C_2$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0