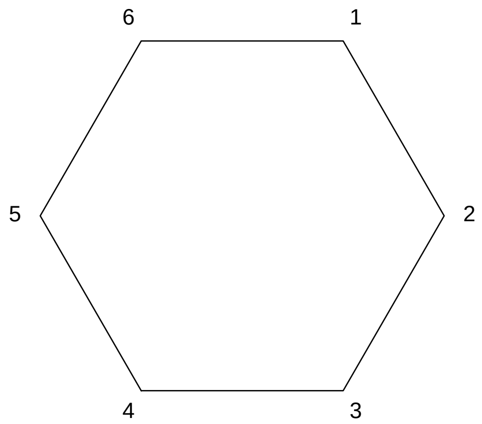
Group Theory

Solutions to Problem Set 7 November 30, 2001

1. A regular hexagon is shown below:

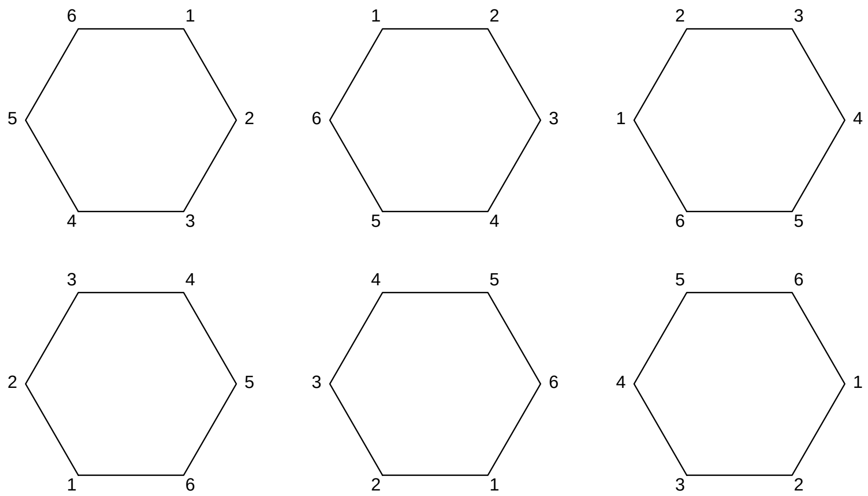


The following notation will be used for the symmetry operations of this hexagon:

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ a_1 & a_2 & a_3 & a_4 & a_5 & a_6 \end{pmatrix},$$

where the first row corresponds to the reference order of the vertices shown in the diagram and the a_i denote the number at the ith vertex *after* the transformation of the hexagon.

The symmetry operations of this hexagon consist of the identity, rotations by angles of $\frac{1}{3}n\pi$ radians, where $n = 1, 2, 3, 4, 5$, three mirror planes which pass through opposite *faces* of the hexagon, and three mirror planes which pass through opposite *vertices* of the hexagon. For the identity and the rotations, the effect on the hexagon is



These operations correspond to

$$E = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & 2 & 3 & 4 & 5 & 6 \end{pmatrix},$$

$$C_6 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 2 & 3 & 4 & 5 & 6 & 1 \end{pmatrix},$$

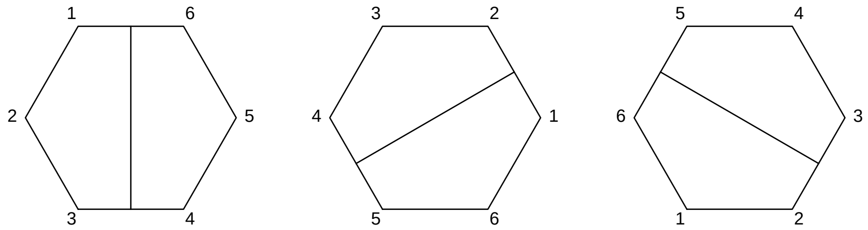
$$C_6^2 = C_3 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 3 & 4 & 5 & 6 & 1 & 2 \end{pmatrix},$$

$$C_6^3 = C_2 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 4 & 5 & 6 & 1 & 2 & 3 \end{pmatrix},$$

$$C_6^4 = C_3^2 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 5 & 6 & 1 & 2 & 3 & 4 \end{pmatrix},$$

$$C_6^5 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 6 & 1 & 2 & 3 & 4 & 5 \end{pmatrix}.$$

The three mirror planes which pass through opposite *faces* of the hexagon are



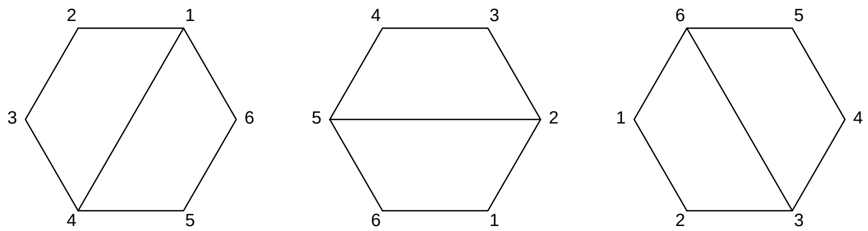
which correspond to

$$\sigma_{v,1} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 6 & 5 & 4 & 3 & 2 & 1 \end{pmatrix} ,$$

$$\sigma_{v,2} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 2 & 1 & 6 & 5 & 4 & 3 \end{pmatrix} ,$$

$$\sigma_{v,3} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 4 & 3 & 2 & 1 & 6 & 5 \end{pmatrix} .$$

Finally, the three mirror planes which pass through opposite *vertices* of the hexagon are



These operations correspond to

$$\sigma_{d,1} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & 6 & 5 & 4 & 3 & 2 \end{pmatrix} ,$$

$$\sigma_{d,2} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 3 & 2 & 1 & 6 & 5 & 4 \end{pmatrix} ,$$

$$\sigma_{d,3} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 5 & 4 & 3 & 2 & 1 & 6 \end{pmatrix} .$$

That these 12 elements do, in fact, form a group is straightforward to verify. The standard notation for this group is C_{6v}.

2. The order n of an element a of a group is defined as the smallest integer such that $a^n = e$. If group elements a and b are in the same class, then there is an element g in the group such that

$$b = g^{-1}ag .$$

The m-fold product of b is then given by

$$b^m = \underbrace{(g^{-1}ag)(g^{-1}ag)\cdots(g^{-1}ag)}_{m\,\text{factors}} = g^{-1}a^m g .$$

If this is equal to the unit element e, we must have

$$g^{-1}a^m g = e ,$$

or,

$$a^m = e .$$

The smallest value of m for which this equality can be satisfied is, by definition, n, the order of a. Hence, two elements in the same class have the same order.

3. For two elements a and b of a group to be in the same class, there must be another group element such that $b = g^{-1}ag$. If the group elements are coordinate transformations, then elements in the same class correspond to the same type of operation, but in coordinate systems related by symmetry operations. This fact, together with the result of Problem 2, allows us to determine the classes of the group of the hexagon.

The identity, as always, is in a class by itself. Although all of the rotations are the same type of operation, not all of these rotations have the same orders: C_6 and C_6^5 have order 6, C_3 and C_3^2 have order 3, and C_2 has order 2. Thus, the 5 rotations belong to *three* different classes.

The two types of mirror planes, $\sigma_{v,i}$ and $\sigma_{d,i}$, *must* belong to different classes since there is no group operation which will transform any of the $\sigma_{v,i}$ to any of the $\sigma_{d,i}$. To do so would require a rotation by an odd multiple of $\frac{1}{6}\pi$, which is not a group element. All of the $\sigma_{v,i}$ are in the same class and all of the $\sigma_{d,i}$ are in the same class, since each is the same type of operation, but in coordinate systems related by symmetry operations (one of the rotations) and, of course, they all have order 2, since each reflection plane is its own inverse.

Hence, there are six classes in this group are

$$\begin{aligned}
E &\equiv \{E\}\,, \\
2C_6 &\equiv \{C_6, C_6^5\}\,, \\
2C_3 &\equiv \{C_3, C_3^2\}\,, \\
C_2 &\equiv \{C_2\}\,, \\
3\sigma_v &\equiv \{\sigma_{v,1}, \sigma_{v,2}, \sigma_{v,3}\}\,, \\
3\sigma_d &\equiv \{\sigma_{d,1}, \sigma_{d,2}, \sigma_{d,3}\}\,.
\end{aligned}$$

4. As there are 6 classes, there are 6 irreducible representations, the dimensions of which must satisfy the sum rule

$$\sum_{k=1}^{6} d_k^2 = 12\,,$$

since $|C_{6v}| = 12$. The only positive integer solutions of this equation are

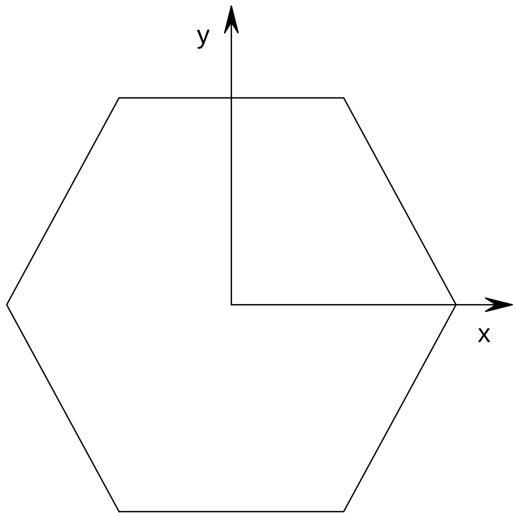
$$d_1 = 1, \quad d_2 = 1, \quad d_3 = 1, \quad d_4 = 1, \quad d_5 = 2, \quad d_6 = 2\,,$$

i.e., there are 4 one-dimensional irreducible representations and 2 two-dimensional irreducible representations.

5. (a) For the identical representation, all of the characters are 1. For the parity representation, the character is 1 for operations which preserve the parity of the coordinate system ("proper" rotations) and -1 for operations which change the parity of the coordinate system ("improper" rotations). Additionally, we can enter immediately the *column* of characters for the class of the unit element. These are equal to the dimensionality of each irreducible representation, since the unit element is the identity matrix with that dimensionality. Thus, we have the following entries for the character table of C_{6v}:

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
Γ_1	1	1	1	1	1	1
Γ_1'	1	1	1	1	-1	-1
Γ_1''	1					
Γ_1'''	1					
Γ_2	2					
Γ_2'	2					

(b) The characters for one of the two-dimensional representations of C_{6v} can be obtained by constructing matrices for operations in analogy with the procedure discussed in Section 3.2 for the equilateral triangle. One important difference here is that we require such a construction only for one element in each class (since the all matrices in a given class have the same trace). We will determine the representations of operations in each class in an (x, y) coordinate system shown below:



Thus, a rotation by an angle ϕ, denoted by $R(\phi)$, is given by the two-dimensional rotational matrix:

$$R(\phi) = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix}.$$

The corresponding character $\chi(\phi)$ is, therefore, simply the sum of the diagonal elements of this matrix:

$$\chi(\phi) = 2\cos\phi\,.$$

We can now calculate the characters for each of the classes composed of rotations:

$$\begin{aligned} \chi(2C_6) &= \chi(\tfrac{1}{3}\pi) = 1\,, \\ \chi(2C_3) &= \chi(\tfrac{2}{3}\pi) = -1\,, \\ \chi(C_2) &= \chi(\pi) = -2\,. \end{aligned}$$

For the two classes of mirror planes, we need only determine the character of one element in each class, which may be chosen at our convenience. Thus, for example, since the representation of

$\sigma_{v,1}$ can be determined directly by inspection:

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

we can obtain the character of the corresponding class as

$$\chi(3\sigma_v) = 0\,.$$

Similarly, the representation of $\sigma_{d,2}$ can also be determined directly by inspection:

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

which yields the character

$$\chi(3\sigma_d) = 0\,.$$

We can now add the entries for this two-dimensional irreducible representations to the character table of C_{6v}:

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
Γ_1	1	1	1	1	1	1
Γ_1'	1	1	1	1	-1	-1
Γ_1''	1					
Γ_1'''	1					
Γ_2	2	1	-1	-2	0	0
Γ_2'	2					

(c) The one-dimensional irreducible representations must obey the multiplication table, since they themselves are representations of the group. In particular, given the products

$$C_3C_3^2 = E, \qquad C_3^3 = E\,,$$

if we denote by α the character of the class $2C_3 = \{C_3, C_3^2\}$, then these products require that

$$\alpha^2 = 1, \qquad \alpha^3 = 1\,,$$

respectively. Thus, we deduce that $\alpha = 1$ for *all* of the one-dimensional irreducible representations. With these additions to the character table, we have

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
Γ_1	1	1	1	1	1	1
Γ_1'	1	1	1	1	-1	-1
Γ_1''	1		1			
Γ_1'''	1		1			
Γ_2	2	1	-1	-2	0	0
Γ_2'	2					

(d) Since the character for all one-dimensional irreducible representations for the class $2C_3 = \{C_3, C_3^2\}$ is unity, the product $C_6C_3 = C_2$ requires that the characters for the classes of C_6 and C_2 are the same in these representations. Since $C_2^2 = E$, this character must be 1 or -1. Suppose we choose $\chi(2C_6) = \chi(C_2) = 1$. Then, the orthogonality of the *columns* of the character table requires that the character for the classes E and $2C_6$ are orthogonal. If we denote by β the character for the class $2C_6$ of the representation Γ_2', we require

$$(1 \times 1) + (1 \times 1) + (1 \times 1) + (1 \times 1) + (2 \times 1) + (2 \times \beta) = 0\,,$$

i.e., $\beta = -3$. But this value violates the requirement that

$$\sum_\alpha n_\alpha |\chi_\alpha|^2 = |G|\,. \qquad (1)$$

Thus, we must choose $\chi(2C_6) = \chi(C_2) = -1$, and our character table becomes

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
Γ_1	1	1	1	1	1	1
Γ_1'	1	1	1	1	-1	-1
Γ_1''	1	-1	1	-1		
Γ_1'''	1	-1	1	-1		
Γ_2	2	1	-1	-2	0	0
Γ_2'	2					

(e) The characters for the classes $2C_6$, $2C_3$, and C_2 of the Γ_2' representation can now be determined by requiring the columns corresponding to these classes to be orthogonal to the column corresponding to the class of the identity. When this is done, we find that the values obtained saturate the sum rule in (1), so the characters corresponding to both classes of mirror planes in this representation must vanish. This enables to complete the entries for the Γ_2' representation:

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
Γ_1	1	1	1	1	1	1
Γ_1'	1	1	1	1	-1	-1
Γ_1''	1	-1	1	-1		
Γ_1'''	1	-1	1	-1		
Γ_2	2	1	-1	-2	0	0
Γ_2'	2	-1	1	2	0	0

The remaining entries are straightforward to calculate. The fact that each mirror reflection has order 2 means that these entries must be either $+1$ or -1. The requirement of orthogonality of columns leaves only one choice:

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
Γ_1	1	1	1	1	1	1
Γ_1'	1	1	1	1	-1	-1
Γ_1''	1	-1	1	-1	1	-1
Γ_1'''	1	-1	1	-1	-1	1
Γ_2	2	1	-1	-2	0	0
Γ_2'	2	-1	1	2	0	0

which completes the character table for C_{6v}.