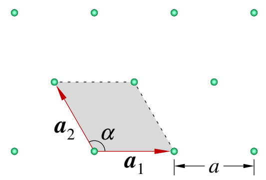
Group Theory

Solutions to Problems in Homework Assignment 09

Spring, 2020

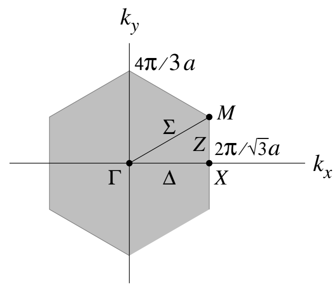
Consider the two-dimensional triangular Bravais lattice (also referred to as the hexagonal Bravais lattice) shown in the figure.



The basic lattice vectors are given by

$$\vec{a}_1 = a\,\vec{e}_x, \;\; \vec{a}_2 = -(a/2)\,\vec{e}_x + (\sqrt{3}a/2)\,\vec{e}_y.$$

1. Find the crystallographic point group of the triangular Bravais lattice. What is the space group of the triangular Bravais lattice in the international system?
2. Construct the character table for the crystallographic point group of the triangular Bravais lattice.
3. Find the basic lattice vectors of the reciprocal lattice of the triangular Bravais lattice. Show that the first Brillouin zone of the triangular Bravais lattice is as given in the following figure



4. Find the point groups for the $\vec{k}$-vectors: $\vec{k}_\Gamma = \vec{0}$, $\vec{k}_X$, and $\vec{k}_M$.
5. Identity the symmetry axes and their point groups in the first Brillouin zone of the triangular Bravais lattice.

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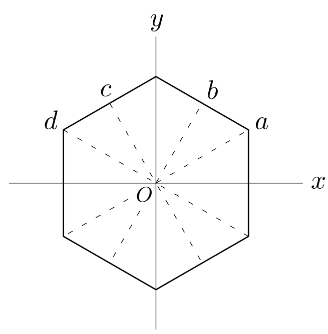
1. The Wigner-Seitz cell of the triangular Bravais lattice is a hexagon. We know that the Wigner-Seitz cell of a Bravais lattice possesses the symmetry of the Bravais lattice. Hence, we can find the point group of the triangular Bravais lattice through finding the symmetry group of a hexagon. We place the hexagon on the xOy plane and use the coordinate system shown in the following figure.



A hexagon possesses the following point symmetry operations.

(i) **The identity E.**

(ii) **The rotation about the Oz-axis through an angle of $2\pi/6$: C_{6z}.**

(iii) **The rotation about the Oz-axis through an angle of $2 \cdot 2\pi/6 = 2\pi/3$: C_{3z}.**

(iv) **The rotation about the Oz-axis through an angle of $3 \cdot 2\pi/6 = 2\pi/2$: C_{2z}.**

(v) **The rotation about the Oz-axis through an angle of $4 \cdot 2\pi/6 = 4\pi/3$: C_{3z}^{-1}.**

(vi) **The rotation about the Oz-axis through an angle of $5 \cdot 2\pi/6$: C_{6z}^{-1}.**

(vii) **The rotation about the Ox-axis through an angle of $2\pi/2$: C_{2x}.**

(viii) **The rotation about the Oy-axis through an angle of $2\pi/2$: C_{2y}.**

(ix) **The rotation about the Oa-axis through an angle of $2\pi/2$: C_{2a}.**

(x) **The rotation about the Ob-axis through an angle of $2\pi/2$: C_{2b}.**

(xi) **The rotation about the Oc-axis through an angle of $2\pi/2$: C_{2c}.**

(xii) **The rotation about the Od-axis through an angle of $2\pi/2$: C_{2d}.**

Thus, the symmetry group of the hexagon is of order 12. Since any two-fold axis in the xOy-plane bisects the angle between the two neighboring two-fold axes in the xOy-plane, the symmetry group of the hexagon is a dihedral group. Since its order is 12, it is denoted by D_6. The symmetry group of the triangular Bravais lattice is thus given by

$$D_6 = \{E, C_{6z}, C_{6z}^{-1}, C_{3z}, C_{3z}^{-1}, C_{2x}, C_{2y}, C_{2z}, C_{2a}, C_{2b}, C_{2c}, C_{2d}\}.$$

The space group of the triangular Bravais lattice in the international system is $P6m$.

2. The transformation matrix for a rotation about the z-axis through an angle of θ is given by

$$R_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

We represent a rotation about an axis in the xOy-plane through $2\pi/2 = \pi$ by a reflection in the xOy-plane with respect to the axis. Then, the transformation matrix of a rotation through an angle of π about an axis that makes an angle of θ with respect to the x-axis is given by

$$S_\theta = \begin{pmatrix} \cos(2\theta) & \sin(2\theta) \\ \sin(2\theta) & -\cos(2\theta) \end{pmatrix}.$$

From the above-given general transformation matrices, we obtain the following transformation matrices for all the elements of D_6

$$R(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad R(C_{6z}) = \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}, \quad R(C_{6z}^{-1}) = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix},$$
$$R(C_{3z}) = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}, \quad R(C_{3z}^{-1}) = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}, \quad R(C_{2x}) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$
$$R(C_{2y}) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad R(C_{2z}) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad R(C_{2a}) = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix},$$
$$R(C_{2b}) = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}, \quad R(C_{2c}) = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}, \quad R(C_{2d}) = \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}.$$

Using the above transformation matrices, we can easily construct the multiplication table for D_6 which is given by

	E	C_{6z}	C_{6z}^{-1}	C_{3z}	C_{3z}^{-1}	C_{2x}	C_{2y}	C_{2z}	C_{2a}	C_{2b}	C_{2c}	C_{2d}
E	E	C_{6z}	C_{6z}^{-1}	C_{3z}	C_{3z}^{-1}	C_{2x}	C_{2y}	C_{2z}	C_{2a}	C_{2b}	C_{2c}	C_{2d}
C_{6z}	C_{6z}	C_{3z}	E	C_{2z}	C_{6z}^{-1}	C_{2a}	C_{2c}	C_{3z}^{-1}	C_{2b}	C_{2y}	C_{2d}	C_{2x}
C_{6z}^{-1}	C_{6z}^{-1}	E	C_{3z}^{-1}	C_{6z}	C_{2z}	C_{2d}	C_{2b}	C_{3z}	C_{2x}	C_{2a}	C_{2y}	C_{2c}
C_{3z}	C_{3z}	C_{2z}	C_{6z}	C_{3z}^{-1}	E	C_{2b}	C_{2d}	C_{6z}^{-1}	C_{2y}	C_{2c}	C_{2x}	C_{2a}
C_{3z}^{-1}	C_{3z}^{-1}	C_{6z}^{-1}	C_{2z}	E	C_{3z}	C_{2c}	C_{2a}	C_{6z}	C_{2d}	C_{2x}	C_{2b}	C_{2y}
C_{2x}	C_{2x}	C_{2d}	C_{2a}	C_{2c}	C_{2b}	E	C_{2z}	C_{2y}	C_{6z}^{-1}	C_{3z}^{-1}	C_{3z}	C_{6z}
C_{2y}	C_{2y}	C_{2b}	C_{2c}	C_{2a}	C_{2d}	C_{2z}	E	C_{2x}	C_{3z}	C_{6z}	C_{6z}^{-1}	C_{3z}^{-1}
C_{2z}	C_{2z}	C_{3z}^{-1}	C_{3z}	C_{6z}^{-1}	C_{6z}	C_{2y}	C_{2x}	E	C_{2c}	C_{2d}	C_{2a}	C_{2b}
C_{2a}	C_{2a}	C_{2x}	C_{2b}	C_{2d}	C_{2y}	C_{6z}	C_{3z}^{-1}	C_{2c}	E	C_{6z}^{-1}	C_{2z}	C_{3z}
C_{2b}	C_{2b}	C_{2a}	C_{2y}	C_{2x}	C_{2c}	C_{3z}	C_{6z}^{-1}	C_{2d}	C_{6z}	E	C_{3z}^{-1}	C_{2z}
C_{2c}	C_{2c}	C_{2y}	C_{2d}	C_{2b}	C_{2x}	C_{3z}^{-1}	C_{6z}	C_{2a}	C_{2z}	C_{3z}	E	C_{6z}^{-1}
C_{2d}	C_{2d}	C_{2c}	C_{2x}	C_{2y}	C_{2a}	C_{6z}^{-1}	C_{3z}	C_{2b}	C_{3z}^{-1}	C_{2z}	C_{6z}	E

Before we find the character table for D_6, we describe some of the properties of D_6, including its classes, nontrivial subgroups, and nontrivial invariant subgroups.

(a) The 6 classes of D_6 are

$$\begin{aligned} &\mathcal{C}_1 = E = \{E\}, && \mathcal{C}_2 = C_2 = \{C_{2z}\}, && \mathcal{C}_3 = 2C_6 = \{C_{6z}, C_{6z}^{-1}\}, \\ &\mathcal{C}_4 = 2C_3 = \{C_{3z}, C_{3z}^{-1}\}, && \mathcal{C}_5 = 3C_2' = \{C_{2x}, C_{2b}, C_{2c}\}, && \mathcal{C}_6 = 3C_2'' = \{C_{2y}, C_{2d}, C_{2a}\}. \end{aligned}$$

(b) The nontrivial subgroups of D_6 are

$$C_2,\ C_3,\ D_2,\ C_6,\ D_3,$$

where

$$\begin{aligned} C_2 &= \{E, C_{2x}\},\ \{E, C_{2y}\},\ \{E, C_{2z}\},\ \{E, C_{2a}\},\ \{E, C_{2b}\},\ \{E, C_{2c}\},\ \{E, C_{2d}\}, \\ C_3 &= \{E, C_{3z}, C_{3z}^{-1}\}, \\ D_2 &= \{E, C_{2x}, C_{2y}, C_{2z}\},\ \{E, C_{2z}, C_{2a}, C_{2c}\},\ \{E, C_{2z}, C_{2b}, C_{2d}\}, \\ C_6 &= \{E, C_{6z}, C_{6z}^{-1}, C_{3z}, C_{3z}^{-1}, C_{2z}\}, \\ D_3 &= \{E, C_{3z}, C_{3z}^{-1}, C_{2x}, C_{2b}, C_{2c}\},\ \{E, C_{3z}, C_{3z}^{-1}, C_{2y}, C_{2a}, C_{2d}\}. \end{aligned}$$

(c) The nontrivial invariant subgroups of D_6 are

$$\begin{aligned} C_2 &= \{E, C_{2x}\}, \\ C_3 &= \{E, C_{3z}, C_{3z}^{-1}\}, \\ C_6 &= \{E, C_{6z}, C_{6z}^{-1}, C_{3z}, C_{3z}^{-1}, C_{2z}\}, \\ D_3 &= \{E, C_{3z}, C_{3z}^{-1}, C_{2x}, C_{2b}, C_{2c}\},\ \{E, C_{3z}, C_{3z}^{-1}, C_{2y}, C_{2a}, C_{2d}\}. \end{aligned}$$

Since D_6 has 6 classes, it has 6 inequivalent irreducible representations. Let n_i be the dimension of the ith inequivalent irreducible representation. We then have

$$\sum_i n_i^2 = g = 12.$$

We take the following solutions to the above equation

$$n_1 = n_2 = n_3 = n_4 = 1,\ n_5 = n_6 = 2.$$

Thus, D_6 has four one-dimensional and two two-dimensional irreducible representations. We first find the characters for the four one-dimensional irreducible representations.

(a) **Identity representation Γ^1.** Let Γ^1 be the identity representation. All the classes have the same character 1 in this representation

$$\chi^1(\mathcal{C}_1) = \chi^1(\mathcal{C}_2) = \chi^1(\mathcal{C}_3) = \chi^1(\mathcal{C}_4) = \chi^1(\mathcal{C}_5) = \chi^1(\mathcal{C}_6) = 1.$$

(b) **One-dimensional irreducible representations Γ^2, Γ^3, and Γ^4.** We next consider the one-dimensional irreducible representations Γ^2, Γ^3, and Γ^4. In consideration that $\chi^p(E) = d_p$, we see that $\chi^p(\mathcal{C}_1) = 1$ for $p = 2$ through 4. From $C_{2x}^2 = C_{2y}^2 = C_{2z}^2 = C_{2a}^2 = C_{2b}^2 = C_{2c}^2 = C_{2d}^2 = E$, we see that

$$\chi^p(\mathcal{C}_2) = \pm 1,\ \chi^p(\mathcal{C}_5) = \pm 1,\ \chi^p(\mathcal{C}_6) = \pm 1,\ p = 2, 3, 4.$$

From $C_{3z}C_{2x} = C_{2b}$, we have

$$\chi^p(\mathcal{C}_4) = 1,\ p = 2, 3, 4.$$

From $C_{2z}C_{3z} = C_{6z}^{-1}$, we have

$$\chi^p(\mathcal{C}_3) = \chi^p(\mathcal{C}_2)\chi^p(\mathcal{C}_4) = \chi^p(\mathcal{C}_2),\ p = 2, 3, 4.$$

From $C_{2z}C_{2y} = C_{2x}$, we have

$$\chi^p(\mathcal{C}_5) = \chi^p(\mathcal{C}_2)\chi^p(\mathcal{C}_6),\ p = 2, 3, 4.$$

i. Γ^2. For Γ^2, we choose $\chi^2(\mathcal{C}_2) = 1$. From $\chi^p(\mathcal{C}_3) = \chi^p(\mathcal{C}_2)$ for $p = 2, 3$, and 4, we have $\chi^2(\mathcal{C}_3) = 1$. If we also choose $\chi^2(\mathcal{C}_6) = 1$, we will then have Γ^2 identical with Γ^1. Thus, we must choose $\chi^2(\mathcal{C}_6) = -1$. We then have $\chi^2(\mathcal{C}_5) = -1$. We have thus obtained the following characters for all the classes of D_6 in Γ^2

$$\chi^2(\mathcal{C}_1) = \chi^2(\mathcal{C}_2) = \chi^2(\mathcal{C}_3) = \chi^2(\mathcal{C}_4) = 1,\ \chi^2(\mathcal{C}_5) = \chi^2(\mathcal{C}_6) = -1.$$

ii. Γ^3. For Γ^3, we can not choose $\chi^3(\mathcal{C}_2) = 1$. If we choose $\chi^3(\mathcal{C}_2) = 1$, we will obtain the characters of the classes in Γ^1 or Γ^2. Hence, we choose $\chi^3(\mathcal{C}_2) = -1$. We can choose either $\chi^3(\mathcal{C}_6) = 1$ or $\chi^3(\mathcal{C}_6) = -1$. For Γ^3, we choose $\chi^3(\mathcal{C}_6) = -1$ and leave $\chi^4(\mathcal{C}_6) = 1$ for Γ^4 together with $\chi^4(\mathcal{C}_2) = -1$. Choosing $\chi^3(\mathcal{C}_2) = -1$ and $\chi^3(\mathcal{C}_6) = -1$, we have $\chi^3(\mathcal{C}_2) = \chi^3(\mathcal{C}_2) = -1$ and $\chi^2(\mathcal{C}_5) = \chi^3(\mathcal{C}_2)\chi^3(\mathcal{C}_6) = 1$. We have thus obtained the following characters for all the classes of D_6 in Γ^3

$$\chi^3(\mathcal{C}_1) = \chi^3(\mathcal{C}_4) = \chi^3(\mathcal{C}_5) = 1,\ \chi^3(\mathcal{C}_2) = \chi^3(\mathcal{C}_3) = \chi^3(\mathcal{C}_6) = -1.$$

iii. Γ^4. As mentioned in the above, we choose $\chi^4(\mathcal{C}_2) = -1$ and $\chi^4(\mathcal{C}_6) = 1$. We then have $\chi^4(\mathcal{C}_3) = \chi^4(\mathcal{C}_2) = -1$ and $\chi^4(\mathcal{C}_5) = \chi^4(\mathcal{C}_2)\chi^4(\mathcal{C}_6) = -1$. We have thus obtained the following characters for all the classes of D_6 in Γ^4

$$\chi^4(\mathcal{C}_1) = \chi^4(\mathcal{C}_4) = \chi^4(\mathcal{C}_6) = 1,\ \chi^4(\mathcal{C}_2) = \chi^4(\mathcal{C}_3) = \chi^4(\mathcal{C}_5) = -1.$$

(c) **Two-dimensional irreducible representations Γ^5 and Γ^6.** Up to now, we have obtained all the characters for the four one-dimensional irreducible representations. We now find the characters in the two two-dimensional irreducible representations.

For the characters in Γ^5 or Γ^6, making use of the orthogonality relation for characters

$$\frac{1}{g}\sum_{T\in D_6} \chi^p(T)^*\chi^q(T) = \delta_{pq}$$

for $q = 5$ or 6 and $p = 1, 2, 3$, and 4, respectively, we have

$$\begin{aligned}
\chi^q(\mathcal{C}_1) + \chi^q(\mathcal{C}_2) + 2\chi^q(\mathcal{C}_3) + 2\chi^q(\mathcal{C}_4) + 3\chi^q(\mathcal{C}_5) + 3\chi^q(\mathcal{C}_6) = 0,\\
\chi^q(\mathcal{C}_1) + \chi^q(\mathcal{C}_2) + 2\chi^q(\mathcal{C}_3) + 2\chi^q(\mathcal{C}_4) - 3\chi^q(\mathcal{C}_5) - 3\chi^q(\mathcal{C}_6) = 0,\\
\chi^q(\mathcal{C}_1) - \chi^q(\mathcal{C}_2) - 2\chi^q(\mathcal{C}_3) + 2\chi^q(\mathcal{C}_4) + 3\chi^q(\mathcal{C}_5) - 3\chi^q(\mathcal{C}_6) = 0,\\
\chi^q(\mathcal{C}_1) - \chi^q(\mathcal{C}_2) - 2\chi^q(\mathcal{C}_3) + 2\chi^q(\mathcal{C}_4) - 3\chi^q(\mathcal{C}_5) + 3\chi^q(\mathcal{C}_6) = 0.
\end{aligned}$$

Adding up the above four equations, we obtain

$$\chi^q(\mathcal{C}_1) + 2\chi^q(\mathcal{C}_4) = 0.$$

Making use of $\chi^q(\mathcal{C}_1) = 2$ for $q = 5$ or 6, we have

$$\chi^q(\mathcal{C}_4) = -1,\ q = 5, 6.$$

Adding up the first two equations in the set of the four equations, we obtain

$$\chi^q(\mathcal{C}_2) = -2\chi^q(\mathcal{C}_3),\ q = 5, 6.$$

Adding up the first and third equations in the set of the four equations, we obtain

$$\chi^q(\mathcal{C}_5) = 0,\ q = 5, 6.$$

Adding up the first and fourth equations in the set of the four equations, we obtain

$$\chi^q(\mathcal{C}_6) = 0,\ q = 5, 6.$$

Setting $p = q$ in the orthogonality relation for characters

$$\frac{1}{g} \sum_{T \in D_6} \chi^p(T)^* \chi^q(T) = \delta_{pq},$$

we have

$$|\chi^q(\mathcal{C}_1)|^2 + |\chi^q(\mathcal{C}_2)|^2 + 2|\chi^q(\mathcal{C}_3)|^2 + 2|\chi^q(\mathcal{C}_4)|^2 + 3|\chi^q(\mathcal{C}_5)|^2 + 3|\chi^q(\mathcal{C}_6)|^2 = 12,\ q = 5, 6.$$

Inserting $\chi^q(\mathcal{C}_1) = 2$ and $\chi^q(\mathcal{C}_4) = -1$ for $q = 5$ or 6 into the above equation yields

$$|\chi^q(\mathcal{C}_2)|^2 + 2|\chi^q(\mathcal{C}_3)|^2 + 3|\chi^q(\mathcal{C}_5)|^2 + 3|\chi^q(\mathcal{C}_6)|^2 = 6,\ q = 5, 6.$$

Inserting $\chi^q(\mathcal{C}_2) = -2\chi^q(\mathcal{C}_3)$ and $\chi^q(\mathcal{C}_5) = \chi^q(\mathcal{C}_6) = 0$ for $q = 5$ or 6, we obtain

$$\chi^q(\mathcal{C}_3) = \pm 1.$$

From $\chi^q(\mathcal{C}_2) = -2\chi^q(\mathcal{C}_3)$, we have

$$\chi^q(\mathcal{C}_2) = \mp 2.$$

We choose $\chi^5(\mathcal{C}_2) = -2$ and $\chi^5(\mathcal{C}_3) = 1$ for Γ^5 and $\chi^5(\mathcal{C}_2) = 2$ and $\chi^5(\mathcal{C}_3) = -1$ for Γ^6. We have thus obtained the following characters for the classes in Γ^5 and Γ^6

$$\chi^5(\mathcal{C}_1) = 2,\ \chi^5(\mathcal{C}_2) = 2,\ \chi^5(\mathcal{C}_3) = -1,\ \chi^5(\mathcal{C}_4) = -1,\ \chi^5(\mathcal{C}_5) = \chi^5(\mathcal{C}_6) = 0,$$
$$\chi^6(\mathcal{C}_1) = 2,\ \chi^6(\mathcal{C}_2) = -2,\ \chi^6(\mathcal{C}_3) = 1,\ \chi^6(\mathcal{C}_4) = -1,\ \chi^6(\mathcal{C}_5) = \chi^6(\mathcal{C}_6) = 0.$$

Collecting the above-obtained results for the characters of the classes, we have the following character table for D_6

	E	C_2	$2C_6$	$2C_3$	$3C_2'$	$3C_2''$
Γ^1	1	1	1	1	1	1
Γ^2	1	1	1	1	-1	-1
Γ^3	1	-1	-1	1	1	-1
Γ^4	1	-1	-1	1	-1	1
Γ^5	2	-2	1	-1	0	0
Γ^6	2	2	-1	-1	0	0

3. To find the basic lattice vectors $\vec{b}_1$ and $\vec{b}_2$ of the reciprocal lattice of the triangular Bravais lattice, we express them in the following form

$$\vec{b}_1 = b_{11}\,\vec{e}_x + b_{12}\,\vec{e}_y,\ \vec{b}_2 = b_{21}\,\vec{e}_x + b_{22}\,\vec{e}_y.$$

For the purpose of deriving general expressions for the basic lattice vectors of the corresponding reciprocal lattice of a two-dimensional Bravais lattice, we also express $\vec{a}_1$ and $\vec{a}_2$ in terms of general coefficients. We have

$$\vec{a}_1 = a_{11}\,\vec{e}_x + a_{12}\,\vec{e}_y,\ \vec{a}_2 = a_{21}\,\vec{e}_x + a_{22}\,\vec{e}_y.$$

Making use of the orthogonality relation $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$, we obtain

$$a_{11}b_{11} + a_{12}b_{12} = 2\pi,\ a_{21}b_{11} + a_{22}b_{12} = 0,$$
$$a_{11}b_{21} + a_{12}b_{22} = 0,\ a_{21}b_{21} + a_{22}b_{22} = 2\pi.$$

Solving these equations, we obtain

$$b_{11} = \frac{2\pi a_{22}}{\Delta},\ b_{12} = -\frac{2\pi a_{21}}{\Delta},\ b_{21} = -\frac{2\pi a_{12}}{\Delta},\ b_{22} = \frac{2\pi a_{11}}{\Delta},$$

where $\Delta = a_{11}a_{22} - a_{12}a_{21}$.

For the triangular Bravais lattice, from the given expressions of the basic lattice vectors in real space, $\vec{a}_1 = a\,\vec{e}_x,\ \vec{a}_2 = -(a/2)\,\vec{e}_x + (\sqrt{3}a/2)\,\vec{e}_y$, we have

$$a_{11} = a,\ a_{12} = 0,\ a_{21} = -a/2,\ a_{22} = \sqrt{3}a/2.$$

We thus have

$$\Delta = a_{11}a_{22} - a_{12}a_{21} = \sqrt{3}a^2/2$$

and

$$b_{11} = \frac{2\pi}{a},\ b_{12} = \frac{2\pi}{\sqrt{3}\,a},\ b_{21} = 0,\ b_{22} = \frac{4\pi}{\sqrt{3}\,a}.$$

$\vec{b}_1$ and $\vec{b}_2$ are then given by

$$\vec{b}_1 = \frac{2\pi}{a}\vec{e}_x + \frac{2\pi}{\sqrt{3}\,a}\vec{e}_y,$$
$$\vec{b}_2 = \frac{4\pi}{\sqrt{3}\,a}\vec{e}_y.$$

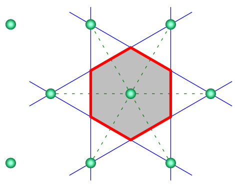
The reciprocal lattice vectors of the triangular Bravais lattice are then given by

$$\vec{K}_m = m_1\vec{b}_1 + m_2\vec{b}_2,\ m_1, m_2 = 0,\ \pm1,\ \pm2,\ \cdots .$$

From the given expressions of the basic lattice vectors of the triangular Bravais lattice, $\vec{a}_1 = a\,\vec{e}_x,\ \vec{a}_2 = -(a/2)\,\vec{e}_x + (\sqrt{3}a/2)\,\vec{e}_y$, we have obtained the following basic lattice vectors of the reciprocal lattice of the triangular Bravais lattice

$$\vec{b}_1 = (2\pi/a)\,\vec{e}_x + (2\pi/\sqrt{3}a)\,\vec{e}_y,\ \vec{b}_2 = (4\pi/\sqrt{3}a)\,\vec{e}_y.$$

From the above expressions of $\vec{b}_1$ and $\vec{b}_2$, we see that the reciprocal lattice of the triangular Bravais lattice is also a triangular Bravais lattice. The first Brillouin zone is the Wigner-Seitz cell of the reciprocal lattice and is constructed in the follow manner



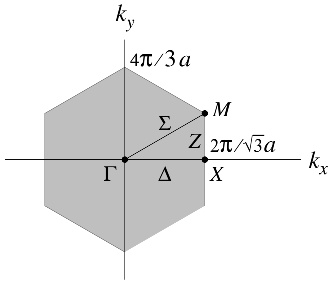
If we choose the k_x-axis to be in the $\vec{e}_y$ direction and the k_y-axis to be in the $\vec{e}_x$ direction, we will have the coordinate system displayed in the figure given in the problem. Let $\hat{k}_x$ and $\hat{k}_y$ denote respectively the unit vectors along the k_x- and k_y-axes. Then the reciprocal lattice vectors are given by

$$\vec{b}_1 = (2\pi/\sqrt{3}a)\,\hat{k}_x + (2\pi/a)\,\hat{k}_y,\ \vec{b}_2 = (4\pi/\sqrt{3}a)\,\hat{k}_x.$$

The reciprocal lattice vectors are given by

$$\vec{K}_{m_1m_2} = m_1\vec{b}_1 + m_2\vec{b}_2 = \frac{2\pi}{\sqrt{3}a}(m_1 + 2m_2)\hat{k}_x + \frac{2\pi}{a}\,m_1\hat{k}_y,\ m_1, m_2 = 0, \pm1, \pm2, \cdots .$$

4. We now find the point groups for the $\vec{k}$-vectors: $\vec{k}_\Gamma = \vec{0}$, $\vec{k}_X$, and $\vec{k}_M$.



(a) $\vec{k}_\Gamma = \vec{0}$**.** For the point $\vec{k}_\Gamma = \vec{0}$, we have

$$R(T)\vec{k}_\Gamma = \vec{k}_\Gamma \text{ for all } T \in D_6.$$

Thus, the point group of $\vec{k}_\Gamma = \vec{0}$ is D_6.

(b) $\vec{k}_X = (2\pi/\sqrt{3}\,a)\hat{k}_x$**.** $\vec{k}_X = (2\pi/\sqrt{3}\,a)\hat{k}_x$ is transformed into the following $\vec{k}$-vectors by the elements of D_6

$$
\begin{aligned}
R(E)\vec{k}_X &= \frac{2\pi}{\sqrt{3}\,a}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{2\pi}{\sqrt{3}\,a}\begin{pmatrix}1\\0\end{pmatrix} = \vec{k}_X,\\
R(C_{6z})\vec{k}_X &= \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}1 & -\sqrt{3}\\ \sqrt{3} & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}1\\ \sqrt{3}\end{pmatrix} = \frac{\pi}{\sqrt{3}\,a}\hat{k}_x + \frac{\pi}{a}\hat{k}_y = \vec{k}_X + \left(-\frac{\pi}{\sqrt{3}\,a}\hat{k}_x + \frac{\pi}{a}\hat{k}_y\right),\\
R(C_{6z}^{-1})\vec{k}_X &= \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}1 & \sqrt{3}\\ -\sqrt{3} & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}1\\ -\sqrt{3}\end{pmatrix} = \frac{\pi}{\sqrt{3}\,a}\hat{k}_x - \frac{\pi}{a}\hat{k}_y = \vec{k}_X - \left(\frac{\pi}{\sqrt{3}\,a}\hat{k}_x + \frac{\pi}{a}\hat{k}_y\right),\\
R(C_{3z})\vec{k}_X &= \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}-1 & -\sqrt{3}\\ \sqrt{3} & -1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}-1\\ \sqrt{3}\end{pmatrix} = -\frac{\pi}{\sqrt{3}\,a}\hat{k}_x + \frac{\pi}{a}\hat{k}_y = \vec{k}_X - \left(\frac{3\pi}{\sqrt{3}\,a}\hat{k}_x - \frac{\pi}{a}\hat{k}_y\right),\\
R(C_{3z}^{-1})\vec{k}_X &= \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}-1 & \sqrt{3}\\ -\sqrt{3} & -1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = -\frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}1\\ \sqrt{3}\end{pmatrix} = -\frac{\pi}{\sqrt{3}\,a}\hat{k}_x - \frac{\pi}{a}\hat{k}_y = \vec{k}_X - \left(\frac{3\pi}{\sqrt{3}\,a}\hat{k}_x + \frac{\pi}{a}\hat{k}_y\right),\\
R(C_{2x})\vec{k}_X &= \frac{2\pi}{\sqrt{3}\,a}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{2\pi}{\sqrt{3}\,a}\begin{pmatrix}1\\0\end{pmatrix} = \frac{2\pi}{\sqrt{3}\,a}\hat{k}_x = \vec{k}_X,\\
R(C_{2y})\vec{k}_X &= \frac{2\pi}{\sqrt{3}\,a}\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{2\pi}{\sqrt{3}\,a}\begin{pmatrix}-1\\0\end{pmatrix} = -\frac{2\pi}{\sqrt{3}\,a}\hat{k}_x = \vec{k}_X - \frac{4\pi}{\sqrt{3}\,a}\hat{k}_x = \vec{k}_X + \vec{K}_{0,-1},\\
R(C_{2z})\vec{k}_X &= \frac{2\pi}{\sqrt{3}\,a}\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{2\pi}{\sqrt{3}\,a}\begin{pmatrix}-1\\0\end{pmatrix} = -\frac{2\pi}{\sqrt{3}\,a}\hat{k}_x = \vec{k}_X - \frac{4\pi}{\sqrt{3}\,a}\hat{k}_x = \vec{k}_X + \vec{K}_{0,-1},\\
R(C_{2a})\vec{k}_X &= \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}1 & \sqrt{3}\\ \sqrt{3} & -1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}1\\ \sqrt{3}\end{pmatrix} = \frac{\pi}{\sqrt{3}\,a}\hat{k}_x + \frac{\pi}{a}\hat{k}_y = \vec{k}_X + \left(-\frac{\pi}{\sqrt{3}\,a}\hat{k}_x + \frac{\pi}{a}\hat{k}_y\right),\\
R(C_{2b})\vec{k}_X &= \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}-1 & \sqrt{3}\\ \sqrt{3} & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}-1\\ \sqrt{3}\end{pmatrix} = -\frac{\pi}{\sqrt{3}\,a}\hat{k}_x + \frac{\pi}{a}\hat{k}_y = \vec{k}_X - \left(\frac{3\pi}{\sqrt{3}\,a}\hat{k}_x - \frac{\pi}{a}\hat{k}_y\right),\\
R(C_{2c})\vec{k}_X &= \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}-1 & -\sqrt{3}\\ -\sqrt{3} & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}-1\\ -\sqrt{3}\end{pmatrix} = -\frac{\pi}{\sqrt{3}\,a}\hat{k}_x - \frac{\pi}{a}\hat{k}_y = \vec{k}_X - \left(\frac{3\pi}{\sqrt{3}\,a}\hat{k}_x + \frac{\pi}{a}\hat{k}_y\right),\\
R(C_{2d})\vec{k}_X &= \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}1 & -\sqrt{3}\\ -\sqrt{3} & -1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\pi}{\sqrt{3}\,a}\begin{pmatrix}1\\ -\sqrt{3}\end{pmatrix} = \frac{\pi}{\sqrt{3}\,a}\hat{k}_x - \frac{\pi}{a}\hat{k}_y = \vec{k}_X - \left(\frac{\pi}{\sqrt{3}\,a}\hat{k}_x + \frac{\pi}{a}\hat{k}_y\right).
\end{aligned}
$$

From the above results, we see that the point group of $\vec{k}_X$ is the subgroup D_2 of D_6 with

$$D_2 = \{E, C_{2x}, C_{2y}, C_{2z}\}.$$

(c) $\vec{k}_M = (2\pi/\sqrt{3}\,a)\hat{k}_x + (2\pi/3a)\hat{k}_y$. $\vec{k}_M = (2\pi/\sqrt{3}\,a)\hat{k}_x + (2\pi/3a)\hat{k}_y = (2\pi/3a)(\sqrt{3}\,\hat{k}_x + \hat{k}_y)$ is transformed into the following $\vec{k}$-vectors by the elements of D_6

The reciprocal lattice vectors are given by

$$\vec{K}_{m_1 m_2} = m_1\vec{b}_1 + m_2\vec{b}_2 = \frac{2\pi}{\sqrt{3}a}(m_1 + 2m_2)\hat{k}_x + \frac{2\pi}{a}\,m_1\hat{k}_y = \frac{2\pi}{3a}[\sqrt{3}(m_1 + 2m_2)\hat{k}_x + 3m_1\hat{k}_y],$$
$$m_1, m_2 = 0, \pm 1, \pm 2, \cdots .$$

$$R(E)\vec{k}_M = \frac{2\pi}{3a}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = \frac{2\pi}{3a}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = \vec{k}_M,$$
$$R(C_{6z})\vec{k}_M = \frac{\pi}{3a}\begin{pmatrix}1 & -\sqrt{3}\\ \sqrt{3} & 1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = \frac{\pi}{3a}\begin{pmatrix}0\\ 4\end{pmatrix} = \frac{4\pi}{3a}\hat{k}_y = \vec{k}_M - \frac{2\pi}{3a}(\sqrt{3}\,\hat{k}_x - \hat{k}_y),$$
$$R(C_{6z}^{-1})\vec{k}_M = \frac{\pi}{3a}\begin{pmatrix}1 & \sqrt{3}\\ -\sqrt{3} & 1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = \frac{2\pi}{3a}\begin{pmatrix}\sqrt{3}\\ -1\end{pmatrix} = \vec{k}_M - \frac{4\pi}{3a}\hat{k}_y,$$
$$R(C_{3z})\vec{k}_M = \frac{\pi}{3a}\begin{pmatrix}-1 & -\sqrt{3}\\ \sqrt{3} & -1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = -\frac{2\pi}{3a}\begin{pmatrix}\sqrt{3}\\ -1\end{pmatrix} = \vec{k}_M - \frac{4\pi}{\sqrt{3}\,a}\hat{k}_x = \vec{k}_M + \vec{K}_{0,-1},$$
$$R(C_{3z}^{-1})\vec{k}_M = \frac{\pi}{3a}\begin{pmatrix}-1 & \sqrt{3}\\ -\sqrt{3} & -1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = -\frac{4\pi}{3a}\begin{pmatrix}0\\ 1\end{pmatrix} = \vec{k}_M - \frac{2\pi}{3a}(\sqrt{3}\,\hat{k}_x + 6\hat{k}_y) = \vec{k}_M + \vec{K}_{-10},$$
$$R(C_{2x})\vec{k}_M = \frac{2\pi}{3a}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = \frac{2\pi}{3a}\begin{pmatrix}\sqrt{3}\\ -1\end{pmatrix} = \vec{k}_M - \frac{4\pi}{3a}\hat{k}_y,$$
$$R(C_{2y})\vec{k}_M = \frac{2\pi}{3a}\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = -\frac{2\pi}{3a}\begin{pmatrix}\sqrt{3}\\ -1\end{pmatrix} = \vec{k}_M - \frac{4\pi}{\sqrt{3}\,a}\hat{k}_x = \vec{k}_M + \vec{K}_{0,-1},$$
$$R(C_{2z})\vec{k}_M = \frac{2\pi}{3a}\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = -\frac{2\pi}{3a}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = -\vec{k}_M = \vec{k}_M - \frac{4\pi}{3a}(\sqrt{3}\,\hat{k}_x + \hat{k}_y),$$
$$R(C_{2a})\vec{k}_M = \frac{\pi}{3a}\begin{pmatrix}1 & \sqrt{3}\\ \sqrt{3} & -1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = \frac{2\pi}{3a}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = \vec{k}_M,$$
$$R(C_{2b})\vec{k}_M = \frac{\pi}{3a}\begin{pmatrix}-1 & \sqrt{3}\\ \sqrt{3} & 1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = \frac{4\pi}{3a}\begin{pmatrix}0\\ 1\end{pmatrix} = \vec{k}_M - \frac{2\pi}{3a}(\sqrt{3}\,\hat{k}_x - \hat{k}_y),$$
$$R(C_{2c})\vec{k}_M = \frac{\pi}{3a}\begin{pmatrix}-1 & -\sqrt{3}\\ -\sqrt{3} & 1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = -\frac{2\pi}{3a}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = -\vec{k}_M = \vec{k}_M - \frac{4\pi}{3a}(\sqrt{3}\,\hat{k}_x + \hat{k}_y),$$
$$R(C_{2d})\vec{k}_M = \frac{\pi}{3a}\begin{pmatrix}1 & -\sqrt{3}\\ -\sqrt{3} & -1\end{pmatrix}\begin{pmatrix}\sqrt{3}\\ 1\end{pmatrix} = -\frac{4\pi}{3a}\begin{pmatrix}0\\ 1\end{pmatrix} = \vec{k}_M - \frac{2\pi}{3a}(\sqrt{3}\,\hat{k}_x + 6\hat{k}_y) = \vec{k}_M + \vec{K}_{-10}.$$

From the above results, we see that E, C_{3z}, C_{3z}^{-1}, C_{2y}, C_{2a}, and C_{2d} are in the point group of $\vec{k}_M$. Thus, the point group of $\vec{k}_M$ is the subgroup D_3 of D_6 with

$$D_3 = \{E, C_{3z}, C_{3z}^{-1}, C_{2y}, C_{2a}, C_{2d}\}.$$

5. Δ, Σ, and Z are the symmetry axes. We now find the point groups of these symmetry axes.

(a) **Symmetry axis Δ.** A $\vec{k}$-vector on Δ can be expressed as

$$\vec{k}_\Delta = \frac{2\pi}{\sqrt{3}\,a}(\xi, 0) = \frac{2\pi}{\sqrt{3}\,a}\xi\hat{k}_x,\ 0 < \xi < 1.$$

Because ξ can take on any arbitrary value in the interval $(0, 1)$, we see that $\vec{k}_\Delta$ is invariant only under the transformations of the elements E and C_{2x} of D_6. Other elements of D_6 do not transform $\vec{k}_\Delta$ into its equivalent positions. Thus, the point group of the symmetry axis Δ is $C_2 = \{E, C_{2x}\}$.

(b) **Symmetry axis Σ.** A $\vec{k}$-vector on Σ can be expressed as

$$\vec{k}_\Sigma = \frac{2\pi}{3a}\xi(\sqrt{3}, 1) = \frac{2\pi}{3a}\xi\big(\sqrt{3}\,\hat{k}_x + \hat{k}_y\big),\ 0 < \xi < 1.$$

Because ξ can take on any arbitrary value in the interval $(0, 1)$, we see that $\vec{k}_\Sigma$ is invariant only under the transformations of the elements E and C_{2a} of D_6. Other elements of D_6 do not transform $\vec{k}_\Delta$ into its equivalent positions. Thus, the point group of the symmetry axis Δ is $C_2 = \{E, C_{2a}\}$.

(c) **Symmetry axis Z.** A $\vec{k}$-vector on Z can be expressed as

$$\vec{k}_Z = \frac{2\pi}{3a}(\sqrt{3}, \xi) = \frac{2\pi}{3a}\big(\sqrt{3}\,\hat{k}_x + \xi\hat{k}_y\big),\ 0 < \xi < 1.$$

Because ξ can take on any arbitrary value in the interval $(0, 1)$, we see that $\vec{k}_\Sigma$ is invariant only under the transformation of the identity element E of D_6. In addition, $\vec{k}_Z$ is transformed by C_{2y} into its equivalent position, $\vec{k}'_Z = \vec{k}_Z + \vec{K}_{0,-1}$. Other elements of D_6 do not transform $\vec{k}_\Delta$ into its equivalent positions. Thus, the point group of the symmetry axis Δ is $C_2 = \{E, C_{2y}\}$.