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The Cayley Graphs of Crystallographic Point Groups Under Hexagonal Crystal System

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ABSTRACT

In chemistry, point groups are used to describe the molecular symmetries of a molecule. Meanwhile, a crystallographic point group is a set of point group that holds at least one point in a fixed position and have some restriction on the rotational symmetries. In this research, the application of graph theory and group theory on the symmetry study of molecules is presented in which the Cayley graph of crystallographic point groups under the hexagonal crystal system is determined. The generators are also computed for groups C_{3h}, C_6, C_{6h}, D_{3h}, C_{6v}, D_6 *and* D_{6h} *and then used to determine the Cayley graph, which is a directed graph representing the group in terms of the generating sets. This research shows that isomorphic crystallographic point groups produce a similar structure to the Cayley graph but different in labelling.*

Keywords: *Cayley graph; crystallographic point group; hexagonal crystal system; symmetry; generating set.*

1. INTRODUCTION

Symmetry has been widely studied in chemical structure and its relation to mathematics. The symmetry of a molecule is described in terms of symmetry elements by the presence of symmetry operations. A symmetry operation is a geometrical transformation or operation, which turns a molecule into an indistinguishable version of itself where it looks the same or there is no difference in the appearance of a molecule before and after performing the operations.

From a chemical perspective, molecules can be highly symmetrical or not symmetrical at all. The fundamental symmetry elements and symmetry operations are important in deciding the symmetry classification of different molecules and it is known as the point groups. Mbah *et al.* have determined the character table of the point group C_{3v} by using matrix representation of the symmetry elements and the orthogonality theorem [1]. The combinations of symmetry operations on a point group would lead to the generation of the other group members. Meanwhile, crystallographic point groups are the product after some restrictions and limitations on the rotational symmetry imposed on point groups.

From the perspective of graph theory, the crystallographic point groups can be presented as Cayley graphs in which consists of a finite number of vertices and edges depending on the choice of the generators. Banaru in 2019 presented the Cayley graphs of the crystallographic groups, which were constructed based on the minimal number of generators [2]. Then, studies on the eigenvalue of Cayley graphs for some symmetric and alternating groups have been

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discussed by Johannes *et al.* [3]. In the same year, Zulkarnain *et al.* had presented the Cayley graph for the non-abelian tensor square of group S_3 [4]. The concept of the Cayley graph is used in this paper to geometrically describe the algebraic structure of some crystallographic point groups. The interest of this research is to determine the Cayley graphs of seven crystallographic point groups under the hexagonal crystal systems.

2. LITERATURE REVIEW

This section presents some definitions and preliminary results, which will be used later to determine the Cayley graph of crystallographic point groups under the hexagonal crystal systems. First, the definition of point groups is discussed.

2.1 Point Group

A point group is a set of symmetry elements with a shape or form that moves through a single point in space, whereas a symmetry element is a geometrical entity such as a line, a plane, or a point where one or more symmetry operation can take place [5]. A symmetry operation is an operation in which leaves an object looking the same or there is no difference in the appearance of a molecule before and after performing the operations. Figure 1 shows how the symmetry operation of C_3, a rotation of $120°$ acts on Tetrachloroplatinate (K_2PtCl_4) molecule which result in an indistinguishable structure of molecule after the operation.

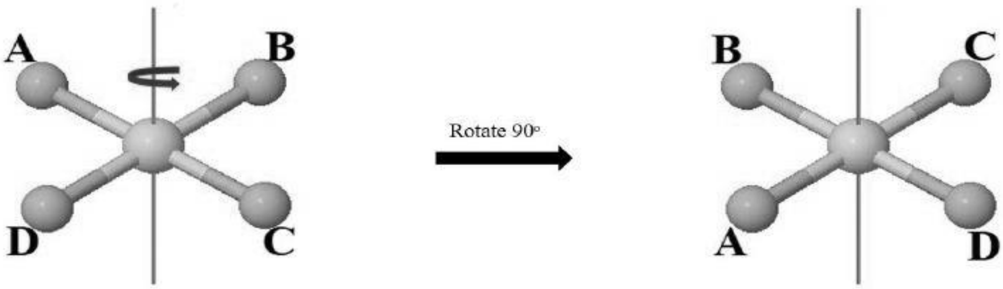

Figure 1: Symmetry operation of C_3 on K_2PtCl_4 molecule

In this research, the Schoenflies notation is employed to describe the symmetry operation of molecules as stated in Table 1.

Table 1: The symmetry operations and Schoendlies notations

Symmetry Operation	Schoenflies Notation	Operation
Identity	E	Represent a rotation of $360°$
Proper rotation	C_n	Proper rotation of $\frac{2\pi}{n}$ and n is the n-fold rotation axis.
Reflection in the vertical plane	σ_v	Reflection in the vertical pane that contains the axis of symmetry
Reflection in the horizontal plane	σ_h	Reflection in the horizontal plane which is perpendicular to the principal axis
Reflection in the diagonal plane	σ_d	Reflection in the diagonal plane that bisects the angle between two vertical planes
Inversion	I	Inversion at the central point

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Improper rotation	S_n	Proper rotation of $\frac{2\pi}{n}$ and the resulting configuration is reflected in a horizontal plane.

The following definition discusses the subdivision of point group, namely crystallographic point groups.

2.2 Crystallographic Point Group

Point groups can be divided into crystallographic point groups and non-crystallographic point groups. In three dimensions, there are 32 crystallographic point groups. Crystallographic point groups can be defined in a finite number of point groups because limitations in rotation and roto inversion are imposed on the internal structure of the crystal in which only certain symmetry elements can occur [6].

Under crystal systems, crystallographic point groups can be divided into seven crystal system with the crystal system being determined by the order of the principal rotation or inversion axis present [7]. For a point group with one principal axis, it belongs to the triclinic, monoclinic, trigonal, tetragonal, or hexagonal crystal system. Meanwhile, orthorhombic and cubic crystal systems have three twofold axes and four threefold axes, respectively.

This research is restricted to crystallographic point groups under the hexagonal crystal systems, which are C_{3h}, C_6, C_{6h}, D_{3h}, C_{6v}, D_6 and D_{6h}. The knowledge of the Cayley graph and crystallographic point groups under the hexagonal crystal system will contribute a lot in understanding and solving the structural problems of a molecule. Previously, Blatov proposes a method for the classification of crystal structures of the chemical compound based on the representation of their graphs [8]. Hence, the characteristic of the hexagonal crystal system which displays a distinguished arrangement that can fill up space is studied in form of the Cayley graph in this research.

The following definitions discuss some fundamental concepts of graph theory that are used throughout this paper.

2.3 Graph

A graph Γ is an ordered pair of disjoint sets $(V(\Gamma), E(\Gamma))$ such that E is a subset of the set V of unordered pairs where $V(\Gamma)$ is the set of vertices and $E(\Gamma)$ is the set of edges [9].

2.4 Isomorphic Graph

Two graphs G and H are isomorphic if H can be obtained from G by relabelling the vertices; that is, if there is a one-to-one correspondence between the vertices of G and those of H, the number of edges joining any pair of vertices in G is equal to the number of edges joining the corresponding pair of vertices in H [10].

2.5 Cayley Graph

For each generating set of set S of a finite group G, there is a directed graph representing the group in terms of the generators in S and is referred to as the Cayley graph. Generating set is a

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subset of a group G that can be expressed as a finite composition of the members of G under the group operation [11].

A different choice for the generating set produces a different Cayley graph. However, the number of edges and vertices is preserved despite changes in the generating set used.

In the following section, a discussion on the method used to determine the generator of certain crystallographic point groups is presented.

3. METHODOLOGY

In this section, the generating sets of generators for all the crystallographic point groups under the hexagonal crystal class are determined. It has been shown that the crystallographic point group C_{3h} is isomorphic to the crystallographic point group C_6, whereas crystallographic point groups D_{3h}, C_{6v}, and D_6 are isomorphic to each other [12].

Generally, crystallographic point groups are classified into eight types that are, C_n, S_n, C_{nv}, C_{nh}, D_{nd}, D_{nh}, T_d, and O_h to analyse their generators in detail. Under the hexagonal crystal system, only C_n, C_{nh}, C_{nv}, D_n, and D_{nh} types are involved and discussed in this research.

For instance, the crystallographic point groups D_{nh} have the symmetry elements of E, C_n, C_2, σ_h and other σ plane. Every crystallographic point group under D_{nh} is generated by C_n and by multiplying C_n with σ_h, which is equal to S_n. Under the hexagonal crystal system, the crystallographic point group $D_{3h} = \{E, C_3, C_3^2, C_2^A, C_2^B, C_2^C, S_3, S_3^5, \sigma_h, \sigma_v^A, \sigma_v^B, \sigma_v^C\}$ can be generated by symmetry operations S_3 and C_2^A. The calculation for D_{3h} is shown as follows:

$$(S_3)(S_3)(S_3)(S_3)(S_3)(S_3) \equiv E,$$

$$(S_3)(S_3) \equiv C_3^2,$$

$$(S_3)(C_2^A) \equiv \sigma_v^B,$$

$$(C_2^A)(S_3) \equiv \sigma_v^C,$$

$$(S_3)(S_3)(S_3) \equiv \sigma_h,$$

$$(C_2^A)(S_3)(S_3) \equiv C_2^C,$$

$$(S_3)(S_3)(S_3)(S_3) \equiv C_3,$$

$$(C_2^A)(S_3)(S_3)(S_3) \equiv \sigma_v^A,$$

$$(S_3)(S_3)(S_3)(S_3)(S_3) \equiv S_3^5,$$

$$(C_2^A)(S_3)(S_3)(S_3)(S_3) \equiv C_2^B.$$

In visualising the Cayley graph, arrows in the edges are used to indicate the permutations of the elements with the generator. The arrows depict how the generator act on the elements or indicate the right-multiplication of the elements with the generators. If the group is generated by more

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than one generating set, then sets of a different number of arrows are used for each generator. Both-sided arrows indicate that the operation is commutative.

By referring to Section 2.5 and the generators obtained, the Cayley graph of the crystallographic point group D_{3h} is determined. The result of successive multiplication of the generators defines the vertices and structure of the graph as shown in Figure 2.

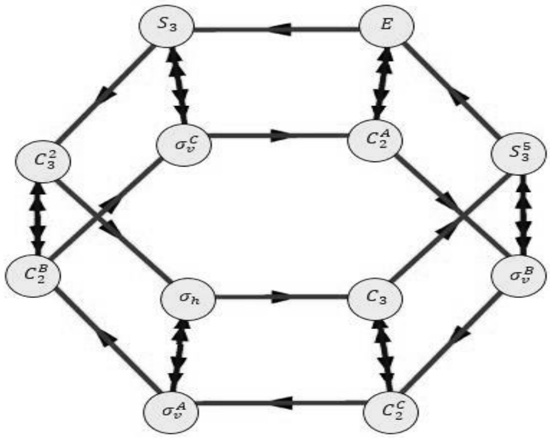

Figure 3: Cayley graph of the crystallographic point group D_{3h}

Table 2 summarised the generators obtained for the crystallographic point groups under the hexagonal crystal system.

Table 2: The generators of the crystallographic point groups under the hexagonal crystal system

Crystallographic Point Group	Elements	Generators
C_{3h}	$E, C_3, C_3^2, S_3, S_3^5, \sigma_h$	S_3
C_6	$E, C_2, C_3, C_3^2, C_6, C_6^5$	C_6
C_{6h}	$E, C_2, C_3, C_6, C_3^2, C_6^5, S_3, S_3^5, S_6, S_6^5, I, \sigma_h$	C_6, σ_h
D_{3h}	$E, C_3, C_3^2, C_2^A, C_2^B, C_2^C, S_3, S_3^5, \sigma_h, \sigma_v^A, \sigma_v^B, \sigma_v^C$	S_3, C_2^A
C_{6v}	$E, C_2, C_3, C_3^2, C_6^5, C_6, \sigma_v^A, \sigma_v^B, \sigma_v^C, \sigma_d^A, \sigma_d^B, \sigma_d^C$	C_6, σ_v^A
D_6	$E, C_2, C_3, C_3^2, C_6^5, C_6, C_2^A, C_2^B, C_2^C, C_2^{A\prime}, C_2^{B\prime}, C_2^{C\prime}$	C_6, C_2^A
D_{6h}	$E, C_3, C_3^2, C_2, C_6, C_6^5, C_2^A, C_2^B, C_2^C, {C_2^A}', {C_2^B}', {C_2^C}'$, $S_3, S_3^5, S_6, S_6^5, I, \sigma_h, \sigma_v^A, \sigma_v^B, \sigma_v^C, \sigma_d^A, \sigma_d^B, \sigma_d^C$	C_6, C_2^A, σ_h

In the next section, the results for the Cayley graph of crystallographic point groups of the hexagonal crystal system are discussed.

4. RESULTS AND DISCUSSION

In this research, the generators of certain crystallographic point groups are determined. Then, Cayley graphs are constructed based on the generators. As stated before, a different choice for the generating set will produce a different Cayley graph. Nevertheless, the number of edges and vertices are preserved despite changes in the generating set used. It is shown in [13] that isomorphic groups will generate the same structure of the graph, but it is different in labelling.

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Hence, this paper will only present the Cayley graphs of C_6, D_{3h}, C_{6h}, and D_{6h} since C_6 is isomorphic with C_{3h} and D_{3h} is isomorphic with C_{6v} and D_6.

First, the Cayley graph of C_6 is presented in Figure 3. Group C_6 can be generated by the element C_6. Here, the single arrows represent the generator C_6.

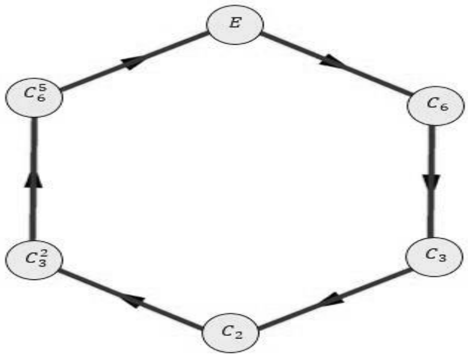

Figure 3: Cayley graph of the crystallographic point group C_6

The Cayley graph of the crystallographic point group C_{3h} is the same as the one presented in Figure 3, where the single arrow represents the generator S_3. The elements of the crystallographic point group C_{3h} corresponding to the nodes of C_6 are listed in Table 3.

Table 3: The nodes and elements of the crystallographic point group C_{3h}

Nodes of C_6	Elements of C_{3h}
E	E
C_6	S_3
C_3	C_3
C_2	σ_h
C_2^3	C_2^3
C_5^5	S_3^5

Next, consider the crystallographic point group C_{6v} and D_6. The Cayley graphs of the crystallographic C_{6v} and D_6 are the same as the one presented in Figure 2, where the single arrow represents the generator C_6, whereas the double arrows represent the generator σ_v^A for both groups. The elements of crystallographic point groups C_{6v} and D_6 corresponding to the nodes of D_{3h} are listed in Table 4.

Table 4: The nodes and elements of the crystallographic point group C_{3h}

Nodes of D_{3h}	Elements of C_{6v}	Elements of D_6
E	E	E
S_3	C_6	C_6
C_3^2	C_3	C_3
σ_h	C_2	C_2
C_3	C_3^2	C_3^2
S_3^5	σ_d^C	C_6^5
C_2^A	σ_v^A	C_2^A
σ_v^B	C_6^5	$C_2^{C'}$
C_2^C	σ_v^B	C_2^B

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σ_v^A	σ_d^A	$C_2^{A'}$
C_2^B	σ_v^C	C_2^C
σ_v^C	σ_d^B	$C_2^{B'}$

Next, the crystallographic point groups C_{6h} can be generated by the elements C_6 and σ_h. The Cayley graph of C_{6h} is represented in Figure 4. Here, the single arrow represents the generator C_6, whereas the double arrows represent the generator σ_h.

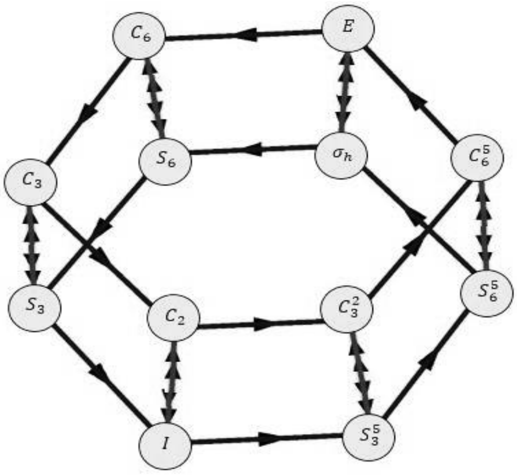

Figure 4: Cayley graph of the crystallographic point group C_{6h}

Lastly, the crystallographic point group D_{6h} can be generated by the elements C_6, C_2^A and σ_h. The Cayley graph of D_{6h} is presented in Figure 5. Here, the single arrow represents the generator C_6, whereas the double and triple arrows represent the generator C_2^A and σ_h, respectively.

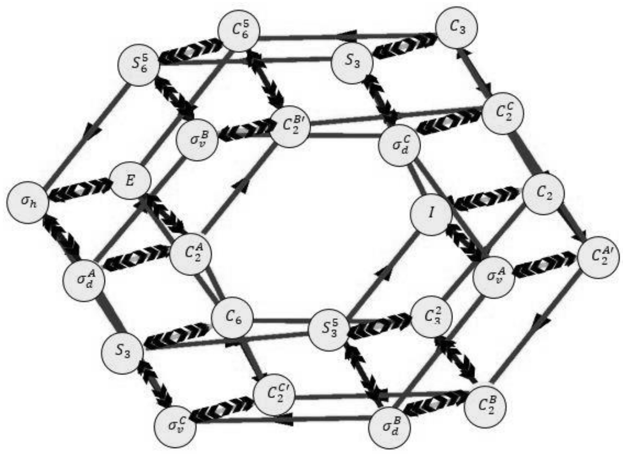

Figure 5: Cayley graph of the crystallographic point group D_{6h}

It can be seen that the Cayley graphs reflect the crystal arrangement of the crystallographic point groups which obey the restriction and limitation imposed by the internal structure of the crystal. Each Cayley graph of the crystallographic point group under a hexagonal crystal system displays a unique motif or arrangement where it can fill the space if the repetitions of such motive or arrangement are carried out. This further substantiates the property of crystallographic point groups under the hexagonal crystal system, which has one principal axis

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of order six. Besides, the results also validate that isomorphic groups generate the same Cayley graph with different labelling of vertices. The similarities include the number of edges and vertices as well as the commutativity of operations on certain generators.

5. CONCLUSION

This paper employs the algebraic concepts in group theory and graph theory on the crystallographic point group in chemistry. The Cayley graphs of the crystallographic point groups are determined for the hexagonal crystal system which are C_{3h}, C_6, C_{6h}, D_{3h}, C_{6v}, D_6, and D_{6h}. The Cayley graphs for the isomorphic groups are found to be similar in structure, having the same number of edges and vertices but different in labelling. This research can be extended to find the Cayley graph for other crystal systems, such as tetragonal, trigonal, and cubic crystal system. Besides, different concepts such as rough approximations and rough edges of the Cayley graph can be studied in this group to analyse their connectivity and graph structure.

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