Proceedings of Science and Mathematics
Faculty of Science, Universiti Teknologi Malaysia
Vol. 23, 2024, page 82-88

Sombor Index of the Cayley Graphs of a Crystallographic Point Group under Hexagonal Crystal System

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Abstract
Crystallography is the science that studies the forms, structures, and arrangements of crystals. It is the experimental determination of the arrangement of atoms in crystalline solids, which is important in materials science, solid-state physics, and many other fields. From a mathematical perspective, symmetry-related phenomena can be described using a variety of mathematical objects. For example, a group can be used to describe the symmetry elements in a crystal. Crystallographic point groups are fundamental in crystallography for describing the symmetry properties of crystals. A crystallographic point group is a set of symmetry operations that keep at least one point fixed in a crystal lattice. They are represented by specific symbols and classified according to the symmetry elements they contain, such as rotation axes, mirror planes, and inversion centers. This research studies the relations of the crystallographic point groups with group theory and graph theory. In this paper, the Cayley graph of a crystallographic point group under hexagonal crystal system is constructed and its Sombor index, which is a vertex-degree-based topological index is determined. The hexagonal crystal system consists of seven point groups that have a single six-fold rotation axis. The focus of this paper is on a crystallographic point group under hexagonal crystal systems, which is C_{6h}. Point group C_{6h} is horizontal mirror plane (σ_h) perpendicular to the principal C_6 axis. Furthermore, the theoretical description of symmetry breaking can be analyzed based on group theory and graph theory by using a Cayley graph. The Cayley graph is a directed graph that represents a finite group *G* in terms of its generating set *S*. A generating set is a subset of a group that can be expressed as a finite composition of its members using group operations. The Cayley graph of the crystallographic point group of C_{6h} are found to be directed, connected and circulant. Based on the structure of the graphs, the Sombor index of the graph is computed in this research.

Keywords: Crystallography; Crystallographic point group; Cayley graph; Sombor index.

1. Introduction

The term "crystallographic" pertains to the examination of how atoms are arranged in crystalline solids and the impact of this arrangement on the material's physical properties [1]. This encompasses the assessment of crystal symmetry and its consequences on diverse physical properties.

A crystallographic point group is a set of point groups that holds at least one point that remains fixed under all symmetry operations and has some rotational symmetry restrictions [2]. Crystallographic point groups can be defined in a finite number of point groups because some restrictions are imposed by the internal structure of the crystal in which only certain symmetry elements can occur. Consequently, rotations and rotoinversions are limited to well-known crystallographic cases of order 1, 2, 3, 4, or 6 [3]. In [3], the seven crystal systems of the crystallographic point groups are triclinic, monoclinic, orthorhombic, trigonal, hexagonal, tetragonal, and cubic.

A point group is a set of symmetry entities that all move through one point in space, while symmetry element is a geometrical unit such as line, a plane, or a point in which one or more symmetry operation can be performed [4]. In [4], a symmetry operation is a geometrical transformation or operation that transforms a molecule into an indistinguishable version of itself in which the appearance of the molecule before and after the operations is the same. According to Ab Hamid [2], the point groups, which are used to classify the symmetry of different molecules, are determined by the fundamental symmetry elements and symmetry operations that they possess.

The crystallographic point groups can be represented as Cayley graphs, with a finite number of vertices and edges depending on the generators used. A Cayley graph is a visual representation of the structure of a group, using a specified set of generators for the group. In [2], graph theory and group theory have been applied to the symmetry study of molecules, and the Cayley graphs of crystallographic point groups under the hexagonal crystal system have been constructed by computing the generators for the point group.

Meanwhile, a topological index is a numerical parameter of a graph that characterizes its topology [5]. Topological indices are calculated based on the molecular graph, which is fundamentally a Cayley graph. One of the topological indices is the Sombor index which is developed in the field of chemical graph theory. In [5], the Sombor index which is a vertex-degree-based graph invariant defined as the sum over all pairs of adjacent vertices of the square root of the sum of their degrees.

Extending the research in [2], this study aims to reconstruct a Cayley graph of the crystallographic point group under the hexagonal crystal system is the crystallographic point group C_{6h}. Then, the Sombor index of the graph is calculated.

2. Basic Concepts

In this section, basic concepts in graph theory, Sombor index of graphs and Cayley graph of groups are included. In addition, the definition of the Cayley graph of the crystallographic point groups are also stated. Lastly, the symmetry elements and symmetry operations of crystallographic point groups C_{6h} are presented.

Definition 2.1 [6] Graph
A graph $\Gamma = (V(\Gamma), E(\Gamma))$ comprises two sets, the vertices, $V(\Gamma)$ and the set of edges, $E(\Gamma)$. Each edge is linked to a set of one or two vertices referred to as its endpoints.

Definition 2.2 [6] Directed Graph
A directed graph, commonly referred to as a digraph, is a graph where a set of vertices or nodes are linked by directed edges. These edges possess a designated direction, signifying a unidirectional relationship between the vertices.

Definition 2.3 [6] Connected Graph
A connected graph is defined by the presence of a path between any two vertices. In simpler terms, it is a graph that cannot be partitioned into two or more disconnected subgraphs. A subgraph is a graph whose vertices and edges are subsets of another graph.

Definition 2.4 [7] Circulant Graph
Let $S = \{a_1, a_2, \ldots, a_k\}$ be a set of integers such that $0 < a_1 < a_2 < \cdots < a_k < \frac{n+1}{2}$. Consider a graph with n vertices labelled $0,1,2, \ldots, n-1$.

A circulant graph $C(n, S)$ is constructed where each vertex of i connected to the vertices $(i + a_1)$ mod n, $(i + a_2)$ mod n, …, $(i + a_k)$ mod n. Each vertex i is adjacent to the vertices obtained by adding the elements of S to i and taking the result modulo n. The set S is called the symbol of the circulant graph $C(n, S)$.

Definition 2.5 [8] Sombor Index of Directed Graph
The Sombor index of directed graph *D* is defined as

$$SO\,(D) = \frac{1}{2} \sum_{uv\,\in A} \sqrt{(d_u^+)^2 + \,(d_v^-)^2}$$

Where V is the set of vertices and A is a subset of the set of ordered pairs of different vertices of D while d_u^+ and d_v^- are the out-degree and in-degree of the vertices *u* and *v* of *D*, respectively.

The out-degree d_u^+ of a vertex *u* of *D* is the number of vertices of *D* that are adjacent from *u*. The in-degree d_v^- of *v* is the number of vertices of *D* adjacent to *v*.

Definition 2.6 [2] Cayley Graph of Crystallographic Point Groups
A Cayley graph of a crystallographic point group is a graphical representation of the group's algebraic structure using vertices and edges. Each vertex in the Cayley graph represents a crystallographic point group element, while each edge represents a group operation that connects one group element to the next.

The elements in crystallographic point group C_{6h} is specified as

$$C_{6h} = \{E, C_2, C_3, C_6, C_3^2, C_6^5, S_3, S_3^5, S_6, S_6^5, I, \sigma_h\}.$$

The symmetry operations of the point group C_{6h} is specified as [10]:
E : Identity,
C_6 : Rotation through $60°$ in the *z* direction,
C_3 : Rotation through $120°$ in the *z* direction,
C_2 : Rotation through $180°$ in the *z* direction,
C_3^2 : Rotation through $240°$ in the *z* direction,
C_6^5 : Rotation through $300°$ in the *z* direction,
I : Inversion,
S_3 : Improper rotation through $120°$ in the *z* direction,
S_3^5 : Improper rotation through $600°$ in the *z* direction,
S_6 : Improper rotation through $60°$ in the *z* direction,
S_6^5 : Improper rotation through $300°$ in the *z* direction,
σ_h : Reflection in the horizontal plane.

3. Research Methodology

The crystallographic point group C_{6h} is generated by the elements C_6 and σ_h. Then, the generating set for crystallographic point group C_{6h} is

$$S = \langle C_6, \sigma_h \rangle = \{E, C_2, C_3, C_6, C_3^2, C_6^5, S_3, S_3^5, S_6, S_6^5, I, \sigma_h\}.$$

The point group C_{6h} has 12 symmetry operations. The elements in point group C_{6h} are

$$C_{6h} = \{E, C_2, C_3, C_6, C_3^2, C_6^5, S_3, S_3^5, S_6, S_6^5, I, \sigma_h\}.$$

The Cayley table of the crystallographic point group C_{6h} is given in Table 3.1.

$*$	E	C_6	C_3	C_2	C_3^2	C_6^5	I	S_3^5	S_6^5	σ_h	S_6	S_3
E	E	C_6	C_3	C_2	C_3^2	C_6^5	I	S_3^5	S_6^5	σ_h	S_6	S_3
C_6	C_6	C_3	C_2	C_3^2	C_6^5	E	S_3^5	S_6^5	σ_h	S_6	S_3	I
C_3	C_3	C_2	C_3^2	C_6^5	E	C_6	S_6^5	σ_h	S_6	S_3	I	S_3^5
C_2	C_2	C_3^2	C_6^5	E	C_6	C_3	σ_h	S_6	S_3	I	S_3^5	S_6^5
C_3^2	C_3^2	C_6^5	E	C_6	C_3	C_2	S_6	S_3	I	S_3^5	S_6^5	σ_h
C_6^5	C_6^5	E	C_6	C_3	C_2	C_3^2	S_3	I	S_3^5	S_6^5	σ_h	S_6
I	I	S_3^5	S_6^5	σ_h	S_6	S_3	E	C_6	C_3	C_2	C_3^2	C_6^5
S_3^5	S_3^5	S_6^5	σ_h	S_6	S_3	I	C_6	C_3	C_2	C_3^2	C_6^5	E
S_6^5	S_6^5	σ_h	S_6	S_3	I	S_3^5	C_3	C_2	C_3^2	C_6^5	E	C_6
σ_h	σ_h	S_6	S_3	I	S_3^5	S_6^5	C_2	C_3^2	C_6^5	E	C_6	C_3
S_6	S_6	S_3	I	S_3^5	S_6^5	σ_h	C_3^2	C_6^5	E	C_6	C_3	C_2
S_3	S_3	I	S_3^5	S_6^5	σ_h	S_6	C_6^5	E	C_6	C_3	C_2	C_3^2

Table 3.1 Cayley table of the crystallographic point group C_{6h}

Next, the Cayley graph of the crystallographic point group C_{6h} is constructed by referring to Table 3.1 and Definition 2.6 (Definition of Cayley graph). Then, based on the graph obtained, the Sombor index of the graph is determined.

4. Results and discussion

4.1. Reconstruction of the Cayley Graphs of Crystallographic Point Groups C_{6h}

Based on Table 3.1 and Definition 2.6 (Definition of Cayley graph), the vertices of the graph is given as

$$V(Cay(C_{6h}, S)) = C_{6h} = \{E, C_2, C_3, C_6, C_3^2, C_6^5, S_3, S_3^5, S_6, S_6^5, I, \sigma_h\}.$$

Then, the Cayley graph of C_{6h} is represented as in Figure 4.1. Here, the single arrow represents generator C_6, and the double arrows represent generator σ_h.

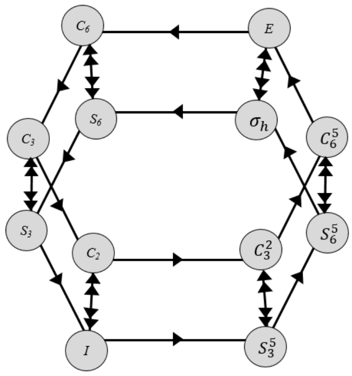

Figure 4.1 Cayley graph of the crystallographic point group C_{6h}

The Cayley graph of the crystallographic point group C_{6h} in Figure 3.2 resulted to be directed, connected and circulant graph. The graph forms a closed loop which is a cycle with no open ends. Each vertex has outgoing edges corresponding to group operations. The direction of edges indicates the transformation from one vertex to another.

Then, the Sombor index of the graph is determined. First, the in-degree and out-degree of each vertex of the graph is presented.

4.2. Sombor Index of the Cayley Graph of Crystallographic Point Group C_{6h}
The Cayley graph of crystallographic point group C_{6h} is given as in Figure 4.1.
Based on the structure of the graph, the in-degree and out-degree of each vertex is determined as summarized in the following Table 4.1.

Vertex	In-degree	Out-degree
E	2	2
C_6	2	2
C_3	2	2
C_2	2	2
C_3^2	2	2
C_6^5	2	2
σ_h	2	2
S_6	2	2
S_3	2	2
I	2	2
S_3^5	2	2
S_6^5	2	2

Table 4.1 The in-degree and out-degree of each vertex of the Cayley graph of crystallographic point group C_{6h}

By Definition 2.5, the Sombor index of $Cay(C_{6h}, S)$ is computed as follows:

$SO\left(Cay(C_{6h},S)\right)$

$$= \frac{1}{2}\Bigg[\sqrt{(d_E^+)^2+\left(d_{C_6}^-\right)^2}+\sqrt{\left(d_{C_6}^+\right)^2+\left(d_{C_3}^-\right)^2}+\sqrt{\left(d_{C_3}^+\right)^2+\left(d_{C_2}^-\right)^2}+\sqrt{\left(d_{C_2}^+\right)^2+\left(d_{C_3^2}^-\right)^2}$$
$$+\sqrt{\left(d_{C_3^2}^+\right)^2+\left(d_{C_6^5}^-\right)^2}+\sqrt{\left(d_{C_6^5}^+\right)^2+(d_E^-)^2}+\sqrt{\left(d_{\sigma_h}^+\right)^2+\left(d_{S_6}^-\right)^2}+\sqrt{\left(d_{S_6}^+\right)^2+\left(d_{S_3}^-\right)^2}$$
$$+\sqrt{\left(d_{S_3}^+\right)^2+(d_I^-)^2}+\sqrt{(d_I^+)^2+\left(d_{S_3^5}^-\right)^2}+\sqrt{\left(d_{S_3^5}^+\right)^2+\left(d_{S_6^5}^-\right)^2}+\sqrt{\left(d_{S_6^5}^+\right)^2+\left(d_{\sigma_h}^-\right)^2}$$
$$+\sqrt{(d_E^+)^2+\left(d_{\sigma_h}^-\right)^2}+\sqrt{\left(d_{\sigma_h}^+\right)^2+(d_E^-)^2}+\sqrt{\left(d_{C_6}^+\right)^2+\left(d_{S_6}^-\right)^2}+\sqrt{\left(d_{S_6}^+\right)^2+\left(d_{C_6}^-\right)^2}$$
$$+\sqrt{\left(d_{C_3}^+\right)^2+\left(d_{S_3}^-\right)^2}+\sqrt{\left(d_{S_3}^+\right)^2+\left(d_{C_3}^-\right)^2}+\sqrt{\left(d_{C_2}^+\right)^2+(d_I^-)^2}+\sqrt{(d_I^+)^2+\left(d_{C_2}^-\right)^2}$$
$$+\sqrt{\left(d_{C_3^2}^+\right)^2+\left(d_{S_3^5}^-\right)^2}+\sqrt{\left(d_{S_3^5}^+\right)^2+\left(d_{C_3^2}^-\right)^2}++\sqrt{\left(d_{C_6^5}^+\right)^2+\left(d_{S_6^5}^-\right)^2}+\sqrt{\left(d_{S_6^5}^+\right)^2+\left(d_{C_6^5}^-\right)^2}\Bigg]$$

$$= \frac{1}{2}\Big[\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}$$
$$+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}$$
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$$+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}$$
$$+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}+\sqrt{(2)^2+(2)^2}\Big]$$

$$= \frac{1}{2}\big[\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}$$
$$+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}+\sqrt{8}\big]$$

$$= \frac{1}{2}\big[24\sqrt{8}\big]$$

$$= 24\sqrt{2}.$$

Conclusion

In this research, the reconstruction of the Cayley graphs of the crystallographic point groups under hexagonal crystal system limited to the crystallographic point groups C_{6h} are presented. The graph is constructed based on the generators $S = \langle C_6, \sigma_h \rangle$ of the groups. The structure of the graph found to be directed, connected and circulant. Next, the computation of the Sombor index of the graph computed on the in-degree and out-degree of each vertex is found to be $SO\ (Cay(C_{6h}, S)) = 24\sqrt{2}$.

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