



# The Conjugacy Class and Conjugacy Class Graph of Crystallographic Point Groups of Order 12 and Above

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## ABSTRACT

In chemistry, crystallographic point group is a set of algebraic groups that maintains at least one point in a fixed position while placing certain restriction on the rotational symmetries. In this research, the application of group theory and graph theory to the symmetry study of a molecule is presented where the conjugacy classes and conjugacy class graphs of crystallographic point groups of order 12 and above are determined. Conjugacy class is a way of classifying the elements of a group such that two elements  $a$  and  $b$  are conjugate if there exists an element  $x$  and given that  $xax^{-1} = b$ . The conjugacy classes obtained are then used to determine the conjugacy class graph in which their vertex set is the set of non-central classes of a group, that is the vertices are connected if the greatest common divisor of the cardinalities of the corresponding vertices is more than one.

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## 1. Introduction

Recent years have shown many studies on symmetry which have been discussed in different branches of science including engineering and structural mechanics. In chemical physics, the symmetry of a molecule or a crystal is described by the existence of symmetry operations performed with respect to the symmetry elements. The study on symmetry elements and symmetry operations by the crystallographers have strengthened the idea in the applications of group theory to crystal systems such as point group and crystallographic point group.

Many ideas of research that have been done on symmetry study and its relation with group theory and graph theory. Previously, Kaveh and Fazli employed the concepts in group theory and graph colouration on symmetric finite elements to factorize an eigenvalue problem to smaller problems [1]. Later, Ghorbani *et al.* [2] have presented some results on symmetry group of cubic polyhedral graphs and found that the order of the symmetry group of such graphs divides 240.

Meanwhile, conjugacy class graph is one of the concepts in graph theory that relate group theory with the symmetry study. This concept was introduced by Bertram in 1990 [3]. Previously, a subgraph of conjugacy class graph of finite groups is presented by Kong and Wang in which the authors discuss the influence of some special vertices on conjugacy class graph [4]. Furthermore, the conjugacy class graphs of point groups of order at most eight were discussed by Abdul Rahman in 2018 where a complete graph denoted as  $K_3$  was obtained for the point group  $C_{4v}$  [5].

This paper is a continuation of [5], therefore, the interest of this research is to obtain the conjugacy class and conjugacy class graph of crystallographic point groups of order 12 and above. Since symmetry operations may be derived from each other by an operation in the same class, the conjugacy class is an essential principle in simplifying the expression of all symmetry operations in a group. Consequently, certain symmetry operations from one crystallographic point group can be grouped using the conjugacy class concept.



## 2. Literature Review

In this section, some mathematical concepts, preliminary results, and basic definitions that are used in this research are stated. Firstly, the definition of point group is discussed.

### Definition 2.1 [6]: Point Group

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 a line, a plane, or a point in which one or more symmetry operation can be performed.

Example of symmetry elements are identity element, plane of symmetry, proper axis, inversion, and rotation-reflection axis or improper axis which are denoted as  $E$ ,  $\sigma$ ,  $C_n$ ,  $I$  and  $S_n$ . Meanwhile, symmetry operations are an operation that 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 is an example showing how the symmetry operation of  $C_3$ , a rotation of  $120^\circ$  acts on a molecule of  $D_{3h}$  namely, Boron Trifluoride ( $BF_3$ ) that result in an indistinguishable structure of molecule after the operation.

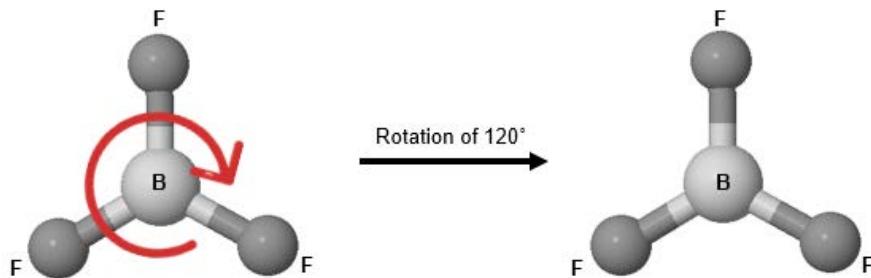


Figure 1. Symmetry operation of  $C_3$  on  $BF_3$

### Definition 2.2 [7]: Crystallographic Point Group

Crystallographic point group is a subgroup of point group with some limitations and restrictions on the rational symmetries are imposed. These limitations will reflect the internal geometric arrangement of molecule and help in classification of the crystallographic point groups into crystal system. In general, crystallographic point groups can be presented in a form of repetitions of the motif in such a way that they completely fill the space. Fundamentally, there are 32 crystallographic point groups in three dimensions with the highest order of 48.

Next, the definition of conjugate of two elements in a group and conjugacy class are stated.

### Definition 2.3 [8]: Conjugate

Elements  $a$  and  $b$  in group  $G$  are conjugate if  $xax^{-1} = b$  or  $xbx^{-1} = a$  for some  $x$  in  $G$ .

When elements of a group are conjugate to each other, they can be grouped and called as conjugacy class.

### Definition 2.4 [8]: Conjugacy class

Let  $a$  be an element of a group  $G$ . The conjugacy class of  $a$  or written as  $cl(a)$  in a group  $G$  is a subset consisting of elements which are all conjugate to each other and can be defined as  $\{xax^{-1} | x \text{ in } G\}$ .

In this research, the number of conjugacy classes in  $G$  is represented by the notation  $K(G)$ .

**Proposition 2.1 [9]** Let  $a$  be an element of a group  $G$ , then  $a$  lies in the centre  $Z(G)$  of  $G$  if and only if the conjugacy class of  $a$  has only one element.

**Proposition 2.2 [9]** Let  $G$  be an abelian group, then  $xax^{-1} = a$  for all  $a$  and  $x$  in  $G$ ; so  $cl(a) = \{a\}$  for all  $a$  in  $G$ .

Next, some fundamental concepts and definitions related to graph are presented.

### Definition 2.5 [10]: Graph

A graph  $G$  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.

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### Definition 2.6 [10]: Complete Graph

A complete graph is a simple graph where any two vertices are adjacent and any complete graph of  $n$  vertices is denoted as  $K_n$ .

### Definition 2.6 [11]: Isomorphic Graph

Two graphs  $G$  and  $H$  are isomorphic if  $H$  can be derived from  $G$  by relabeling the vertices; that is, if the vertices of  $G$  and  $H$  have a one-to-one correspondence, with the number of edges joining each pair of vertices in  $G$  equaling the number of edges joining the corresponding pair of vertices in  $H$ .

### Definition 2.7 [3]: Conjugacy Class Graph

A conjugacy class graph is a graph whose vertices  $V = \{v_1, \dots, v_n\}$  are the non-central conjugacy classes of a group  $G$ , and two vertices are connected if their cardinalities are not coprime and their greatest common divisor (gcd) of the cardinalities is greater than one.

In the following section, methods to obtain conjugacy class and conjugacy class graph are presented.

### 3. Methodology

Previously, it has been proven that crystallographic point groups  $D_{3d}$ ,  $D_{3h}$ ,  $C_{6v}$ , and  $D_6$  are isomorphic to non-abelian dihedral group of order 12,  $D_6$  [12]. Besides, the crystallographic point groups  $T_d$  and  $O$  are isomorphic to symmetric group of order 24. Consequently, by using the Definition 2.6, the conjugacy class graphs of all the isomorphic groups are found to be similar in structure but different in labelling.

Next, the conjugacy classes and conjugacy class graphs of crystallographic point groups of order 12 and above are determined.

First, consider  $T = \{E, C_2(z), C_2(y), C_2(x), C_3^A, C_3^B, C_3^C, C_3^D, C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}\}$ . The elements of group  $T$  are determined from the symmetry operations that act on the symmetry elements of group  $T$  and described in Schoenflies notation. For example,  $C_2(z)$  is a proper rotation of  $180^\circ$  about the z-axis. The conjugacy classes of element  $C_2(z)$  in  $T$  are found by using the Definition 2.4 and Proposition 2.2 as follows:

$$\begin{aligned} \text{Let } x = E, xax^{-1} &= (E)C_2(z)(E) = C_2(z), \\ \text{let } x = C_2(z), xax^{-1} &= (C_2(z))C_2(z)(C_2(z)) = C_2(z), \\ \text{let } x = C_2(y), xax^{-1} &= (C_2(y))C_2(z)(C_2(y)) = C_2(z), \\ \text{let } x = C_2(x), xax^{-1} &= (C_2(x))C_2(z)(C_2(x)) = C_2(z), \\ \text{let } x = C_3^A, xax^{-1} &= (C_3^A)C_2(z)(C_3^{2A}) = C_2(x), \\ \text{let } x = C_3^B, xax^{-1} &= (C_3^B)C_2(z)(C_3^{2B}) = C_2(x), \\ \text{let } x = C_3^C, xax^{-1} &= (C_3^C)C_2(z)(C_3^{2C}) = C_2(x), \\ \text{let } x = C_3^D, xax^{-1} &= (C_3^D)C_2(z)(C_3^{2D}) = C_2(x), \\ \text{let } x = C_3^{2A}, xax^{-1} &= (C_3^{2A})C_2(z)(C_3^A) = C_2(y), \\ \text{let } x = C_3^{2B}, xax^{-1} &= (C_3^{2B})C_2(z)(C_3^B) = C_2(y), \\ \text{let } x = C_3^{2C}, xax^{-1} &= (C_3^{2C})C_2(z)(C_3^C) = C_2(y), \\ \text{let } x = C_3^{2D}, xax^{-1} &= (C_3^{2D})C_2(z)(C_3^D) = C_2(y). \end{aligned}$$

Thus,  $\text{cl}(C_2(z)) = \{C_2(z), C_2(y), C_2(x)\}$ . The same method is used to determine the conjugacy classes for the other elements of  $T$ . The conjugacy classes of  $T$  are listed as follows:

- i.  $\text{cl}(E) = \{E\}$ ,
- ii.  $\text{cl}(C_2(z)) = \{C_2(z), C_2(y), C_2(x)\}$ ,
- iii.  $\text{cl}(C_3^A) = \{C_3^A, C_3^B, C_3^C, C_3^D\}$ ,
- iv.  $\text{cl}(C_3^{2A}) = \{C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}\}$ .

It is found that  $K(T) = 4$  and  $|Z(T)| = 1$ . In order to generate the conjugacy class graph of crystallographic point group  $T$ , the result on conjugacy classes of group  $T$  is applied to the Definition 2.7, in which two distinct vertices are connected given that the greatest common divisor of the size of the conjugacy classes is greater than one. In this case, the  $\text{gcd}(|\text{cl}(C_2(z))|, |\text{cl}(C_3^A)|) = \text{gcd}(3,4) =$

$1, \gcd(|\text{cl}(C_2(z))|, |\text{cl}(C_3^{2A})|) = \gcd(3,4) = 1$  and  $\gcd(|\text{cl}(C_3^A)|, |\text{cl}(C_3^{2A})|) = \gcd(4,4) = 4$ . Therefore, only vertices of  $\text{cl}(C_3^A)$  and  $\text{cl}(C_3^{2A})$  are connected and the conjugacy class graph of  $T$  is presented in Figure 1.



Figure 2. Conjugacy class graph of crystallographic point group  $T$

In the following section, the conjugacy classes and conjugacy class graphs for all the groups are discussed.

#### 4. Results and Discussion

In this section, the conjugacy classes of all the crystallographic point groups of order 12 and above are found by using the definition of conjugacy classes and as discussed in the previous section. Table 1 summarizes the conjugacy classes,  $K(G)$  and number of central conjugacy classes,  $|Z(G)|$  for all the crystallographic point groups of order 12 and above.

Table 1. The conjugacy classes and the number of  $Z(G)$  for the crystallographic point groups of order 12 and above.

Groups	Symmetry Elements	Conjugacy Classes	$K(G)$	No. Of $Z(G)$
$T$	$E, C_2(z), C_2(y), C_2(x), C_3^A, C_3^B, C_3^C, C_3^D, C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}$	$\text{cl}(E) = \{E\}, \text{cl}(C_2(z)) = \{C_2(z), C_2(y), C_2(x)\}, \text{cl}(C_3^A) = \{C_3^A, C_3^B, C_3^C, C_3^D\}, \text{cl}(C_3^{2A}) = \{C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}\}.$	4	1
$D_{3d}$	$E, C_3, C_3^2, C_2^A, C_2^B, C_2^C, I, S_6, S_6^5, \sigma_d^A, \sigma_d^B, \sigma_d^C$	$\text{cl}(E) = \{E\}, \text{cl}(C_3) = \{C_3, C_3^2\}, \text{cl}(C_2^A) = \{C_2^A, C_2^B, C_2^C\}, \text{cl}(I) = \{I\}, \text{cl}(S_6) = \{S_6, S_6^5\}, \text{cl}(\sigma_d^A) = \{\sigma_d^A, \sigma_d^B, \sigma_d^C\}$	6	2
$D_{3h}$	$E, C_3, C_3^2, C_2^A, C_2^B, C_2^C, S_3, S_3^5, \sigma_h, \sigma_v^A, \sigma_v^B, \sigma_v^C$	$\text{cl}(E) = \{E\}, \text{cl}(C_3) = \{C_3, C_3^2\}, \text{cl}(C_2^A) = \{C_2^A, C_2^B, C_2^C\}, \text{cl}(\sigma_h) = \{\sigma_h\}, \text{cl}(S_3) = \{S_3, S_3^5\}, \text{cl}(\sigma_v^A) = \{\sigma_v^A, \sigma_v^B, \sigma_v^C\}$	6	2
$C_{6v}$	$E, C_2, C_3, C_3^2, C_6, C_6^5, \sigma_v^A, \sigma_v^B, \sigma_v^C, \sigma_d^A, \sigma_d^B, \sigma_d^C$	$\text{cl}(E) = \{E\}, \text{cl}(C_3) = \{C_3, C_3^2\}, \text{cl}(C_6) = \{C_6, C_6^5\}, \text{cl}(C_2) = \{C_2\}, \text{cl}(\sigma_d^A) = \{\sigma_d^A, \sigma_d^B, \sigma_d^C\}, \text{cl}(\sigma_v^A) = \{\sigma_v^A, \sigma_v^B, \sigma_v^C\}$	6	2
$D_6$	$E, C_2, C_3, C_3^2, C_6, C_6^5, C_2^A, C_2^B, C_2^C, C_2^D, C_2^{A'}, C_2^{B'}, C_2^{C'}$	$\text{cl}(E) = \{E\}, \text{cl}(C_3) = \{C_3, C_3^2\}, \text{cl}(C_6) = \{C_6, C_6^5\}, \text{cl}(C_2) = \{C_2\}, \text{cl}(C_2^A) = \{C_2^A, C_2^B, C_2^C\}, \text{cl}(C_2^{A'}) = \{C_2^{A'}, C_2^{B'}, C_2^{C'}\}.$	6	2
$D_{4h}$	$E, C_2, C_4, C_4^3, C_2^A, C_2^B, C_2^{A'}, C_2^{B'}, I, S_4, S_4^3, \sigma_h, \sigma_v^A, \sigma_v^B, \sigma_d^A, \sigma_d^B$	$\text{cl}(E) = \{E\}, \text{cl}(\sigma_d^A) = \{\sigma_d^A, \sigma_d^B\}, \text{cl}(I) = \{I\}, \text{cl}(\sigma_h) = \{\sigma_h\}, \text{cl}(C_4) = \{C_4, C_4^3\}, \text{cl}(C_2^A) = \{C_2^A, C_2^B\}, \text{cl}(S_4) = \{S_4, S_4^3\}, \text{cl}(C_2) = \{C_2\}, \text{cl}(C_2^{A'}) = \{C_2^{A'}, C_2^{B'}\}, \text{cl}(\sigma_v^A) = \{\sigma_v^A, \sigma_v^B\}.$	10	4
$D_{6h}$	$E, C_2, C_3, C_3^2, C_6, C_6^5, C_2^A, C_2^B, C_2^C, C_2^D, C_2^{A'}, C_2^{B'}, C_2^{C'}, I, S_6, S_6^5, S_3, S_3^5, \sigma_h, \sigma_v^A, \sigma_v^B, \sigma_v^C, \sigma_d^A, \sigma_d^B, \sigma_d^C$	$\text{cl}(E) = \{E\}, \text{cl}(I) = \{I\}, \text{cl}(C_2) = \{C_2\}, \text{cl}(\sigma_h) = \{\sigma_h\}, \text{cl}(C_3) = \{C_3, C_3^2\}, \text{cl}(C_6) = \{C_6, C_6^5\}, \text{cl}(S_3) = \{S_3, S_3^5\}, \text{cl}(C_2^A) = \{C_2^A, C_2^B, C_2^C\}, \text{cl}(C_2^{A'}) = \{C_2^{A'}, C_2^{B'}, C_2^{C'}\}, \text{cl}(S_6) = \{S_6, S_6^5\}, \text{cl}(\sigma_d^A) = \{\sigma_d^A, \sigma_d^B, \sigma_d^C\}, \text{cl}(\sigma_v^A) = \{\sigma_v^A, \sigma_v^B, \sigma_v^C\}.$	12	4
$T_h$	$E, C_2(z), C_2(y), C_2(x), C_3^A, C_3^B, C_3^C, C_3^D, C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}, S_6^A, S_6^B, S_6^C, S_6^D, S_6^{5A}, S_6^{5B}, S_6^{5C}, S_6^{5D}, I, \sigma_h(xy), \sigma_h(xz), \sigma_h(yz)$	$\text{cl}(E) = \{E\}, \text{cl}(I) = \{I\}, \text{cl}(C_3^A) = \{C_3^A, C_3^B, C_3^C, C_3^D\}, \text{cl}(S_6^A) = \{S_6^A, S_6^B, S_6^C, S_6^D\}, \text{cl}(S_6^{5A}) = \{S_6^{5A}, S_6^{5B}, S_6^{5C}, S_6^{5D}\}, \text{cl}(C_3^{2A}) = \{C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}\}, \text{cl}(C_2(z)) =$	8	2

		$\{C_2(z), C_2(y), C_2(x)\}, \text{cl}(\sigma_h(xy)) = \{\sigma_h(xy), \sigma_h(xz), \sigma_h(yz)\}.$		
$T_d$	$E, C_2(z), C_2(y), C_2(x), C_3^A, C_3^B, C_3^C, C_3^D, C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}, \sigma_d^A, \sigma_d^B, \sigma_d^C, \sigma_d^{A'}, \sigma_d^{B'}, \sigma_d^{C'}, \sigma_d^A, S_4^A, S_4^B, S_4^C, S_4^{3A}, S_4^{3B}, S_4^{3C}$	$\text{cl}(E) = \{E\}, \text{cl}(C_3^A) = \{C_3^A, C_3^B, C_3^C, C_3^D, C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}\}, \text{cl}(\sigma_d^A) = \{\sigma_d^A, \sigma_d^B, \sigma_d^C, \sigma_d^{A'}, \sigma_d^{B'}, \sigma_d^{C'}\}, \text{cl}(S_4^A) = \{S_4^A, S_4^B, S_4^C, S_4^{3A}, S_4^{3B}, S_4^{3C}\}, \text{cl}(C_2(z)) = \{C_2(z), C_2(y), C_2(x)\}.$	5	1
$O$	$E, C_2(z), C_2(y), C_2(x), C_3^A, C_3^B, C_3^C, C_3^D, C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}, C_2^A, C_2^B, C_2^C, C_2^{A'}, C_2^{B'}, C_2^{C'}, C_4(z), C_4(y), C_4(x), C_4(z)^3, C_4(y)^3, C_4(x)^3$	$\text{cl}(E) = \{E\}, \text{cl}(C_3^A) = \{C_3^A, C_3^B, C_3^C, C_3^D, C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}\}, \text{cl}(C_2^A) = \{C_2^A, C_2^B, C_2^C, C_2^{A'}, C_2^{B'}, C_2^{C'}\}, \text{cl}(C_2(z)) = \{C_2(z), C_2(y), C_2(x)\}, \text{cl}(C_4(z)) = \{C_4(z), C_4(y), C_4(x), C_4(z)^3, C_4(y)^3, C_4(x)^3\}$	5	1
$O_h$	$E, C_2(z), C_2(y), C_2(x), C_3^A, C_3^B, C_3^C, C_3^D, C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}, C_2^A, C_2^B, C_2^C, C_2^{A'}, C_2^{B'}, C_2^{C'}, C_4^A, C_4^B, C_4^C, C_4^{3A}, C_4^{3B}, C_4^{3C}, I, \sigma_h(xy), \sigma_h(xz), \sigma_h(yz), S_6^A, S_6^B, S_6^C, S_6^D, S_6^{5A}, S_6^{5B}, S_6^{5C}, S_6^{5D}, \sigma_d^A, \sigma_d^B, \sigma_d^C, \sigma_d^{A'}, \sigma_d^{B'}, \sigma_d^{C'}, S_4^A, S_4^B, S_4^C, S_4^{3A}, S_4^{3B}, S_4^{3C}.$	$\text{cl}(E) = \{E\}, \text{cl}(I) = \{I\}, \text{cl}(C_2(z)) = \{C_2(z), C_2(y), C_2(x)\}, \text{cl}(C_3^A) = \{C_3^A, C_3^B, C_3^C, C_3^D, C_3^{2A}, C_3^{2B}, C_3^{2C}, C_3^{2D}\}, \text{cl}(C_2^A) = \{C_2^A, C_2^B, C_2^C, C_2^{A'}, C_2^{B'}, C_2^{C'}\}, \text{cl}(C_4^A) = \{C_4^A, C_4^B, C_4^C, C_4^{3A}, C_4^{3B}, C_4^{3C}\}, \text{cl}(S_4^A) = \{S_4^A, S_4^B, S_4^C, S_4^{3A}, S_4^{3B}, S_4^{3C}\}, \text{cl}(\sigma_d^A) = \{\sigma_d^A, \sigma_d^B, \sigma_d^C, \sigma_d^{A'}, \sigma_d^{B'}, \sigma_d^{C'}\}, \text{cl}(\sigma_h(xy)) = \{\sigma_h(xy), \sigma_h(xz), \sigma_h(yz)\}, \text{cl}(S_6^A) = \{S_6^A, S_6^B, S_6^C, S_6^D, S_6^{5A}, S_6^{5B}, S_6^{5C}, S_6^{5D}\}.$	10	2

Next, by using the definition of conjugacy class graph, the conjugacy class graphs of all 12 groups are presented. For crystallographic point group  $C_{6h}$ , the conjugacy class graph cannot be generated as it is an abelian group. By using the Proposition 2.1, the number of non-central conjugacy class of  $C_{6h}$  is zero.

First, the conjugacy class graph of  $D_{3d}$  of order 12 is shown in Figure 2. The number of non-central conjugacy class of  $D_{3d}$  is four.

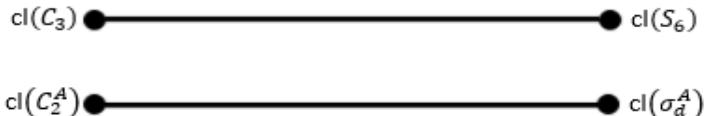


Figure 2. Conjugacy class graph of crystallographic point group  $D_{3d}$

Since the crystallographic point group  $D_{3d}$  is isomorphic to  $D_{3h}$ ,  $D_6$ , and  $C_{6v}$ , the conjugacy class graph of all the groups is similar in structure but different in vertices labelling. The vertices of  $D_{3h}$ ,  $C_{6v}$ , and  $D_6$  corresponding to the vertices of  $D_{3d}$  are listed in Table 2.

Table 2. The vertices of  $D_{3h}$ ,  $C_{6v}$ , and  $D_6$  corresponding to the vertices of  $D_{3d}$

Vertices of $D_{3d}$	Vertices of $D_{3h}$	Vertices of $D_6$	Vertices of $C_{6v}$
$\text{cl}(C_3)$	$\text{cl}(C_3)$	$\text{cl}(C_3)$	$\text{cl}(C_3)$
$\text{cl}(S_6)$	$\text{cl}(S_3)$	$\text{cl}(S_6)$	$\text{cl}(S_6)$
$\text{cl}(C_2^A)$	$\text{cl}(C_2^A)$	$\text{cl}(C_2^A)$	$\text{cl}(\sigma_d^A)$
$\text{cl}(\sigma_d^A)$	$\text{cl}(\sigma_v^A)$	$\text{cl}(C_2^{A'})$	$\text{cl}(\sigma_v^A)$

Next, the conjugacy class graph of crystallographic point group  $D_{4h}$  of order 16 is presented in Figure 3. The number of non-central conjugacy class of  $D_{4h}$  is six.

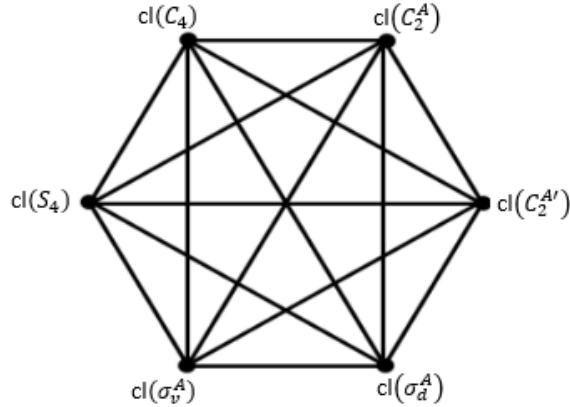


Figure 3. Conjugacy class graph of crystallographic point group  $D_{4h}$

Crystallographic point group  $D_{4h}$  produces a complete conjugacy class graph, denoted as  $K_6$ . Next, the conjugacy class graph of crystallographic point group  $D_{6h}$  of order 24 is presented in Figure 4. The number of non-central conjugacy class of  $D_{6h}$  is eight.

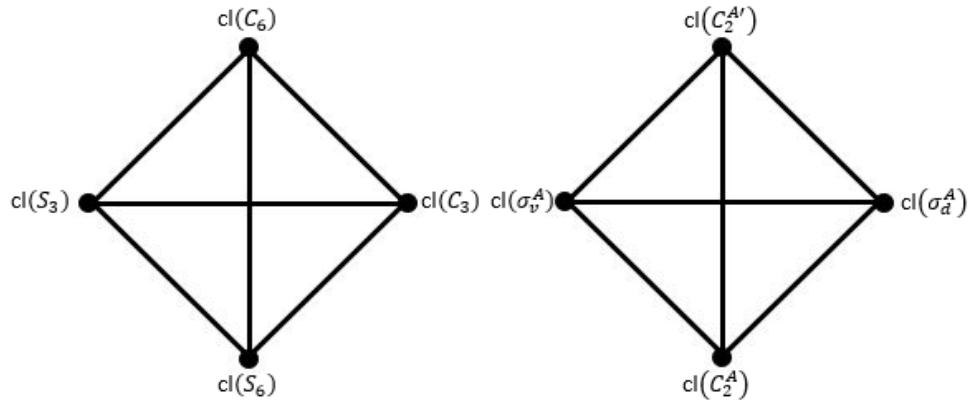


Figure 4. Conjugacy class graph of crystallographic point group  $D_{6h}$

Next, the conjugacy class graph of crystallographic point group  $T_h$  of order 24 is presented in Figure 5. The number of non-central conjugacy class of  $T_h$  is six.

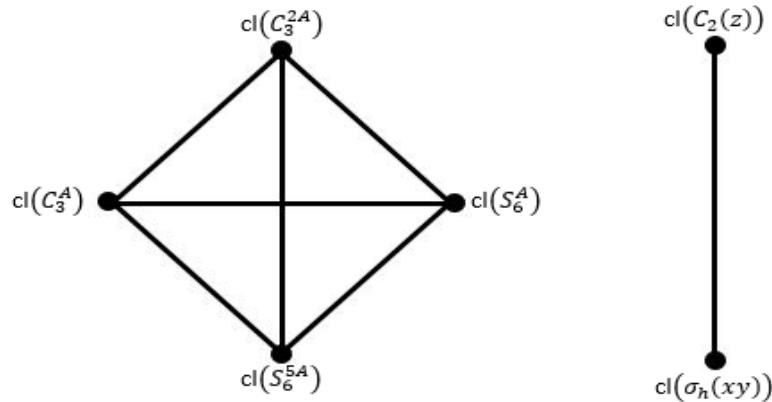


Figure 5. Conjugacy class graph of crystallographic point group  $T_h$

Next, the conjugacy class graph of crystallographic point group  $T_d$  of order 24 is presented in Figure 6. The number of non-central conjugacy class of  $T_d$  is four.

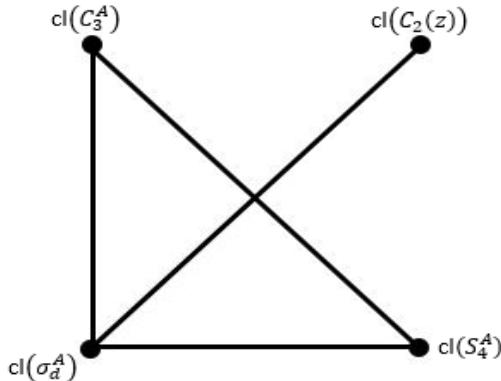


Figure 6. Conjugacy class graph of crystallographic point group  $T_d$

Since the crystallographic point group  $T_d$  is isomorphic to  $O$ , the conjugacy class graph for both groups is similar in structure but different in vertices labelling. The vertices of  $O$  corresponding to the vertices of  $T_d$  are listed in Table 3.

Table 3. The vertices of  $O$  corresponding to the vertices of  $T_d$

Vertices of $T_d$	Vertices of $O$
$\text{cl}(C_3^A)$	$\text{cl}(C_3^A)$
$\text{cl}(\sigma_d^A)$	$\text{cl}(C_2^A)$
$\text{cl}(S_4^A)$	$\text{Cl}(C_2(z))$
$\text{cl}(C_2(z))$	$\text{Cl}(C_2(z))$

Lastly, the conjugacy class graph of crystallographic point group  $O_h$  of order 48 is presented in Figure 7. The number of non-central conjugacy class of  $O_h$  is eight.

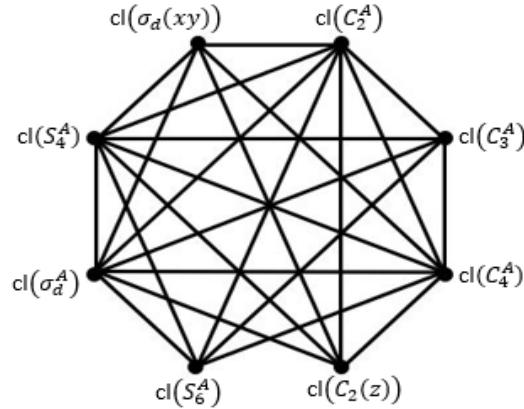


Figure 7. Conjugacy class graph of crystallographic point group  $O_h$

The result shows that only crystallographic point groups  $T$  and  $D_{4h}$  generate a complete graph denoted as  $K_2$  and  $K_6$  respectively, in which all the vertices are connected. The application of the conjugacy classes in crystallographic point groups is essential in simplifying the expression of all the symmetry operations in a group since the operations in the same conjugacy class are equivalent and can be generated from each other by the same operation. By way of explanation, Table 1 shows the symmetry operations of the same conjugacy classes which are equivalent and can be derived from each other by the same generating set. Besides, the conjugacy class graphs obtained in this

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research represent a model of the pairwise relation between the conjugacy classes of the crystallographic point group.

## 5. Conclusion

In this research, the conjugacy classes for crystallographic point groups of order 12 and above are determined. Next, the conjugacy class graphs are presented. It is proven that the crystallographic point group  $C_{6h}$  consists of singleton sets with zero non-central conjugacy classes, hence the conjugacy class graph of  $C_{6h}$  cannot be generated. For isomorphic groups, the conjugacy class graphs are found to be similar in number of vertices and connectivity but different in labelling. Furthermore, it is found that only crystallographic point group  $T$  and  $D_{4h}$  produce complete graphs and denoted as  $K_2$  and  $K_6$  respectively. This research can be extended to determine the chromatic number, clique number, and the denominating number of the conjugacy class graph of crystallographic point groups.

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