Finite Representation for Seven Crystal Systems

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ABSTRACT

The developments of some rigid mathematical criteria of symmetry are required in order to make the idea of a molecular system as useful as possible. The first consideration was on the kinds of symmetry elements that a molecule may have and the symmetry operations generated by the symmetry elements presented in symmetry groups. The classification of finite symmetry groups in R^3 has important applications in crystallography. Many chemical substances from crystals and their structures take the forms of crystalline lattices. This study present the classification of chemistry point groups according to the seven crystal systems. The generators can be described in terms of chemistry point groups' elements or abstract symmetry group elements accordingly. By using GAP, the possible relations between the set of generators and the finite representations for corresponding abstract groups of crystallographic point groups were determined. From the result of finite presentations of abstract symmetry groups, the generators and relations of chemistry point groups can be described using the symmetry elements of point groups.

Keywords: *Finite symmetry groups, generators, relations, finite representations.*

Introduction

Symmetry groups play a main role in chemistry, especially in molecular vibration (Cotton, 1990). Vibration modes of benzene (Wilson, 1934), methyl acetylene (Meister *et. al*, 1943), water (Sarmin & Mohamad, 2004), and ammonia (Sarmin *et. al*, 2004) are examples that can be treated quite simply by group theory. Symmetry groups are the groups that are most often encountered by most chemists and by many physicists. The point group theory (and symmetry) provides the mathematical basis for interpretation of the spectra of molecules. The various vibration modes of a molecule can be categorized in terms of their behavior with respect to the symmetry elements of the molecule. Classification of point groups, group representations, character tables and structure can have physical meanings to chemists and physicists.

Finite rotation groups of rigid bodies and crystallographic point groups which are also known as lattice point groups or point groups in chemistry, are two types of symmetry point groups. A finite symmetry point group cannot contain translations, glides or screws and so arguing as before, such a group must fix some point which we may as well considered as the origin. This study will classified the idgroup, generators and relation in order to determine the finite representation group of seven holohedry

32 Crystallographic Point Groups

There are at least 32 point groups in chemistry which can be used to determine the finite symmetry subgroups of Sym_n using the isomorphic relation. Gilbert (2004) shows this classification of finite symmetries in R^3 has important application in crystallography. Many chemical substances from crystal and their structure take the form of crystalline lattices. A crystal lattice is always finite, but in order to study its symmetries, we create a mathematical model by extending this crystal lattice to infinity. Common salt form a cubic crystalline lattice has the orthogonal vector of the same length. A subgroup of O(3) that leaves a crystalline lattice invariant is called **crystallographic point groups.**

In three dimensions there are 32 such point groups, 30 of which are relevant to chemistry. Their classification is based on the Schönflies notation. A crystal consist an ordered 3D repetition of a fundamental unit (the asymmetric unit), which may be one molecule or several molecules (all the same of several kinds). This order array consists of a large number of unit cells (effectively, an infinite number) that fit together to fill the space and that are defined by three translation vectors. The point groups determine the classes of mathematically possible lattice known as crystal system and it is conventional to divide the crystal classes into seven crystals which are triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral or trigonal, hexagonal and cubic.

In Hestenes (2002), a set of generators for each of the seven holohedry is determined and identified with lattice vectors which are the symmetry vectors that generate the lattice. Since all the chemistry point groups are subgroups of O_h and D_{6h}, the generators of these crystallographic point groups can be generated from the generators of O_h and D_{6h}. Geometry algebra also describes possible relation between the set of generators for each of the seven diholohedry. We will determine the mapping between the elements in symmetric operations in the crystallographic point groups to corresponding generators in certain crystal system.

Seven Crystal Systems

A crystal consists of an ordered 3D repetition of a fundamental unit (the asymmetric unit), which may be one molecule or several molecules (all the same of several kinds). This order array consists of a large number of unit cells (effectively, an infinite number) that fit together to fill space and that are defined by three translation vectors. The termini of these vectors repeated over and over, form an array of points called the crystal lattice (Cotton, 1990). There are seven crystal systems as listed in the following

a) **Triclinic** - The least symmetrical of the crystal systems. No face has the same dimensions as any other and none of the faces is at right angles to any of the others.
b) **Monoclinic** - One of the most common crystal systems. No pair of faces is the same length, breadth or height as any other.
c) **Orthorhombic** - This system has flattened sides that look like table tops. The three faces are unequal, but they are all at right angles to one another.
d) **Tetragonal** - This form is more elongated than the cube. The crystals have three faces at right angles to one another, but only two are equal in length, breadth and height.
e) **Rhombohedral** or trigonal – Has three-dimensional shape that is similar to a cube that has been compreesed to one side. Its form is considered prismatic, as all faces are parallel to each other. The faces that are not square are called "rhombi". A rhombohedral crystal has six faces or rhombi, 12 edges and 8 vertices. If all of the non-obtuse internal angles of the faces are equal, it can be called a trigonal trarezohedron.
f) **Hexagonal** – Has four crystallographic axes consisting of three equal horizontal or equatorial axes at $120°$, and one vertical axis that are perpendicular to the other three.
g) **Cubic** - Crystal that is essentially cube-shaped, like dice, with three pairs of sides the same length, breadth and height. Some cubic crystals may have developed further into 8- or 12-sided shapes, but these still belong to the cubic system. These crystals are also called isometric crystals.

The subdivision corresponds to an arrangement of the point groups into families of subgroups, as indicated in Figure 1 and the largest group in each system is called holohedry of the system. In Hestenes (2002), a set of generators for each of the seven holohedry is determined and identified with lattice vectors which are the symmetry vectors that generate the lattice. Since all the chemistry point groups are subgroups of O_h and D_{6h}, the generators of these crystallographic point groups can be generated from the generators of O_h and D_{6h}. Geometry algebra also describes possible relation between the set of generators for each of the seven diholohedry (the versor groups of the holohedry).

Relation of one system to another is described by the subgroup relations among the holohedry, as shown in Figure 2. The point groups shown in each holohedry are the generators of each crystal systems. Table 1 has sets of such generators arranged to show the simple relations among them. Note that the orthogonal vectors **a**, **c** can be chosen to be the same for each system, and there are three distinct choices for the remaining vector **b**. Actually from the generators for O_h and D_{6h} the generators of all other crystallographic point groups can be generated because all the groups are subgroups of O_h and D_{6h}, as shown in Figure 1. We have determined all possible point symmetry groups for 3-dimensional objects. However, an infinite number of different objects with the same symmetry groups, for a symmetry group describe a relation among identical parts of an object without saying anything about the nature of those parts (Hestenes, 2002).

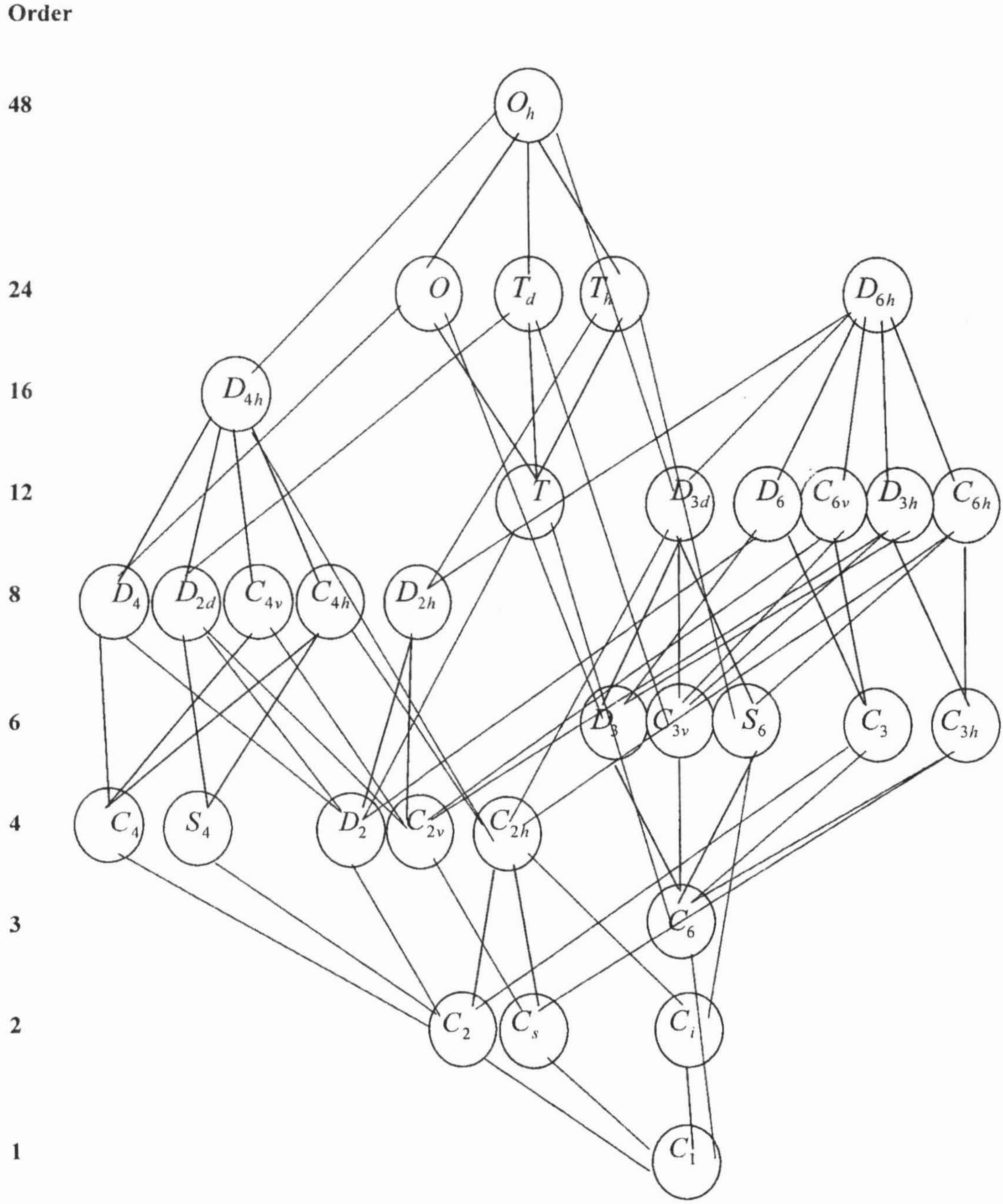

Figure 1 **Subgroup relations among the 32 crystallographic point groups. Darklines connectgroup in the same crystal system (Hestenes, 2002)**

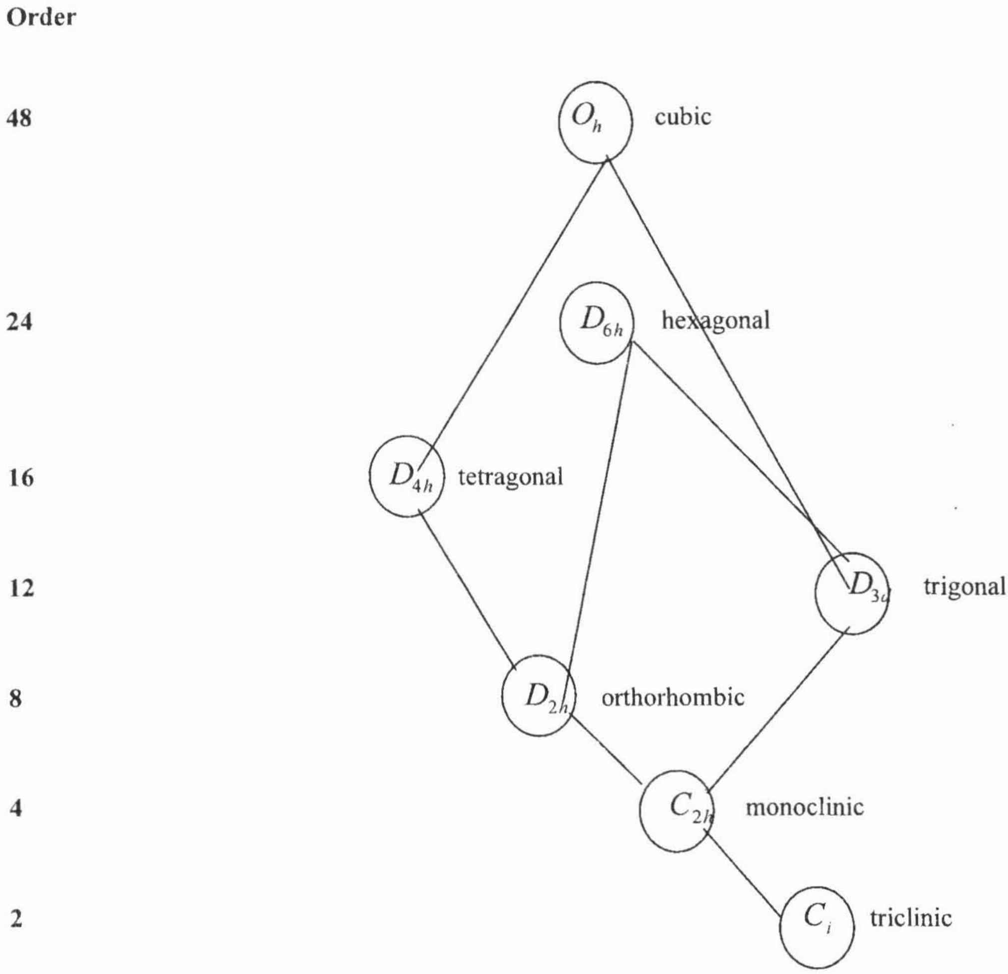

Figure 2 Subgroup Relations for the Seven Holohedry or Crystal Systems

According to the Figure 2, each of the seven crystal system was generated by one of the point groups in their crystal class. In Table 4.10, the generators of the point groups that represent each crystal class is given in terms of vectors. Here we give the group theoretical representation of each of the holohedry groups using finite presentation groups of its corresponding abstract group types. Since all the chemistry point groups are subgroups of O_h and D_{6h}, the generators of these crystallographic point groups can be generated from the generators of O_h and D_{6h}. The finite presentation group of the abstract group for D_{6h} can be applied to describe the generators of D_{6h} and their properties.

Finite Representation Group

The idea of a group representation is to form a group by giving a set of generators for the group and certain equation or relation that we want the generators to satisfy and want the group to be as free as it possibly can be on the generators with these relations (Fraleigh, 2000). The finite representations for six crystal systems are listed in Table 1. All of these finite representations were determined by using GAP. GAP stands for **Groups, Algorithms and Programming**.But we are enabling to determine the finite presentation of the holohedry group $O_h \approx Sym_4 \times Z_2$ using the usual procedures applied to the other holohedry groups.

Table 1: Finite Representation for Generators of Crystal System

Crystal System	Generator of Crystal System	Abstract Group	Finite Representation (GAP)
Triclinic	C_i	Z_2	$G = \langle a : a^2 = e \rangle$
Monoclinic	C_{2h}	Dih_2	$G = \langle a,b : a^2 = b^2 = e, (ab)^{-1}ba = e \rangle$
Orthorhombic	D_{2h}	$Dih_2 \times Z_2$	$G = \langle a,b,c : a^2 = b^2 = c^2 = e; (ab)^{-1}ba = (ac)^{-1}ca = (bc)^{-1}cb = e \rangle$
Trigonal	D_{3d}	$Dih_6 = Dih_3 \times Z_2$	$G = \langle a,b,c : a^2 = c^3 = e; (ab)^{-1}bac^{-2} = (ac)^{-1}cac^{-1} = e; (bc)^{-1}cb = e; b^2c^{-1} = e \rangle$
Tetragonal	D_{4h}	$Dih_4 \times Z_2$	$G = \langle a,b,c,d : a^2 = c^2 = d^2 = e, b^2c^{-1} = e; (ab)^{-1}bac^{-1} = e; (ac)^{-1}ca = (ad)^{-1}da = (bc)^{-1}cb = (bd)^{-1}db = (cd)^{-1}dc = e \rangle$
Hexagonal	D_{6h}	$Dih_6 \times Z_2$	$G = \langle a,b,c,d : a^2 = c^3 = e; b^2c^{-1} = e; (ab)^{-1}bac^{-2} = (ac)^{-1}cac^{-1} = e; (ad)^{-1}da = (bc)^{-1}cb = (bd)^{-1}db = (cd)^{-1}dc = e \rangle$
Cubic	O_h	$Sym_4 \times Z_2$	—

Table 2: Finite Representation for Seven Crystal System

Crystal System	Generator of Crystal System	Abstract Group	Finite Representation
Triclinic	C_i	Z_2	$G = \langle a : a^2 = e \rangle$
Monoclinic	C_{2h}	Dih_2	$G = \langle a,b : a^2 = b^2 = e, ab = ba \rangle$
Orthorhombic	D_{2h}	$Dih_2 \times Z_2$	$G = \langle a,b,c : a^2 = b^2 = c^2 = e; ab = ba; ac = ca; cd = dc \rangle$
Trigonal	D_{3d}	$Dih_6 = Dih_3 \times Z_2$	$G = \langle a,b,c : a^2 = b^6 = e; ba = b^5; b^2a = ab^4 \rangle$
Tetragonal	D_{4h}	$Dih_4 \times Z_2$	$G = \langle a,b,c,d : a^2 = c^2 = d^2 = e; b^2 = c; ab = ba; ac = ca; ad = da; bc = cb; bd = dc; cd = dc \rangle$
Hexagonal	D_{6h}	$Dih_6 \times Z_2$	$G = \langle a,b,c,d : a^2 = c^3 = e; b^2 = c; ba = abc^2; ca = {}^3; ab = ba; ac = ca; ad = da; bc = cb; bd = db; cd = dc \rangle$
Cubic	O_h	$Sym_4 \times Z_2$	—

Conclusion

The seven crystal systems for the 32 crystallographic point groups as listed are classified in terms of the unit cell dimension and the required symmetry element. Each crystal systems present different unit cell dimension and different fold axes which are represent the different 3D Bravais Lattices in each of the crystal system. The visualization of all point groups in each crystal systems shows that each point groups were extend under the symmetry operations in each crystal systems. End of these operations, the visualization will shows the figure that present the generator of each crystal systems (holohedry) and the representation of finite group for each of the crystal systems.

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