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PHASE TRANSITIONS IN CRYSTALLINE SOLIDS I: AUTOMORPHISMS AND EXTENSIONS OF CRYSTALLOGRAPHIC AND ICOSAHEDRAL POINT GROUPS

TRANSITION DE PHASE DES CRISTAUX SOLIDES I: AUTOMORPHISMES ET EXTENSIONS DE GROUPES PONCTUELS CRISTALLO-GRAPHIQUES ET ICOSAÉDRAUX

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RÉSUMÉ

De nombreux cristaux présentant de l'intérêt pour le Programme nucléaire canadien peuvent subir des transitions de phase dans leur champ d'application. Au cours de cette transition de phase, une représentation du groupe spatial du polymorphe à plus haute symétrie s'affaiblit et permet ainsi de produire la transition.

Le présent rapport est le premier d'une série intéressant les propriétés (influencées par la théorie des groupes) de la transition de phase des cristaux. L'objet de la recherche est d'identifier tous les modes mous spectroscopiquement actifs des 230 groupes ponctuels de l'espace euclidien. L'identification de ces modes mous permettra l'examen détaillé de la transition de phase des cristaux présentant de l'intérêt pour le Programme nucléaire canadien et aidera à l'optimalisation des propriétés des cristaux.

Dans le présent rapport, on examine les propriétés (influencées par la théorie des groupes) des structures cristallines et de la transition de phase. On démontre que le problème de l'extension d'un groupe se réduit au problème de la détermination de ses automorphismes. On tire les groupes d'automorphismes des groupes ponctuels cristallographiques et icosaédraux à l'aide d'une présentation constante (régulière).

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ABSTRACT

Many crystalline materials of interest to the Canadian Nuclear Program have the potential to undergo phase transitions in their range of application. During such phase transitions, a representation of the space group of the higher symmetry polymorph softens to induce the transition.

This report is the first in a series of reports concerned with the group-theoretic properties of phase transitions in crystalline materials. The object of the research is to identify all spectroscopically-active soft modes for the 230 three-dimensional space groups. Identification of these soft modes will enable a detailed examination of phase transitions in materials of interest to the Canadian Nuclear Program and aid in the optimization of material properties.

In this report, the group-theoretic properties of crystal structures and phase transitions are reviewed. It is demonstrated that the problem of extending a group reduces to that of determining its automorphisms. The automorphism groups of the crystallographic and icosahedral point groups are derived using a consistent presentation.

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CONTENTS

1. INTRODUCTION

A crystalline phase of a material can exist in one or more polymorphs. The polymorph corresponding to the equilibrium structure for a given set of conditions is the polymorph with the lowest free energy under these conditions.

Should the conditions change (e.g., pressure, temperature changes) then a different polymorph may become stabilized relative to the original structure. This will occur if the new polymorph has a lower free energy under the changed conditions. If thermodynamic equilibrium is to be restored, then the crystal must undergo a transition to the lowest free energy. The transition that connects the two polymorphs is known as a phase transition.

Many crystalline materials that are of interest to the Canadian Nuclear Program have the potential to undergo phase transitions in their range of application. Examples of materials exhibiting phase transitions are:

UO_2 [1]	A fuel material,
ThO_2 [2]	A fuel material for advanced fuel cycles,
ZrO_2 [3]	An insulating material with low neutron cross-section, and
BeO [4]	A moderator material for high-temperature application.

During the phase transition a representation of the space group of the higher symmetry polymorph softens to induce the transition. In the case of structural phase transitions, the transition is induced by the softening of a vibrational or librational mode.

This report is part of a series of reports concerned with the group-theoretic properties of phase transitions in crystalline materials. The object of the research is to identify all spectroscopically-active soft modes for the 230 three-dimensional space groups. Identification of these soft modes will enable a detailed examination of phase transitions in experimental facilities such as DUALSPEC [5]. These studies will aid in the optimization of materials of interest to the Canadian Nuclear Program.

In this report, we will review the group-theoretic properties of crystal structures and phase transitions. We will demonstrate that the problem of extending a group reduces to that of determining its automorphisms. Finally, we will derive the automorphism groups of the crystallographic and icosahedral point groups with a consistent presentation.

2. CRYSTALLOGRAPHIC GROUPS

2.1 Bravais Lattices

2.1.1 One-Dimensional

There is a single one-dimensional lattice. This consists of a single row of equally-spaced points.

2.1.2 Two-Dimensional

There are five two-dimensional lattices. All of the lattices are primitive, except one rectangular lattice that is body-centered. The two-dimensional lattices are given in Table 1.

Table 1
The Five Two-Dimensional Lattices

System	Number of Lattices in System	Nature of Axes and Angles
Oblique	1	$a \neq b$ $\gamma \neq 90°$
Rectangular	2	$a \neq b$ $\gamma = 90°$
Square	1	$a = b$ $\gamma = 90°$
Hexagonal	1	$a = b$ $\gamma = 120°$

2.1.3 Three-Dimensional

There are fourteen three-dimensional lattices. They are listed in Table 2. The lattice symbols used in Table 2 refer to the different types of lattice as follows:

A, B, or C	Centered on one pair of opposite faces of the unit cell as well as having points at the corners,
F	All faces centered, in addition to points at the corners,
I	Body centered, in addition to points at the corners,
P	Primitive (points only at the corners), except rhombohedral,
R	Primitive rhombohedral.

Table 2
The Fourteen Three-Dimensional Lattices

System	Number of Lattices in System	Lattice Symbols	Nature of Axes and Angles
Triclinic	1	P	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90°$
Monoclinic	2	P, B (or C)	$a \neq b \neq c$ $\alpha = \beta = 90° \neq \gamma$
Orthorhombic	4	P, C, I, F	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$
Tetragonal	2	P, I	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$
Cubic	3	P, I, F	$a = b = c$ $\alpha = \beta = \gamma = 90°$
Trigonal	1	R	$a = b = c$ $\alpha = \beta = \gamma < 120°, \neq 90°$
Hexagonal	1	P	$a = b \neq c$ $\alpha = \beta = 90°, \gamma = 120°$

2.1.4 Four-Dimensional

There are 64 four-dimensional lattices. The reader is referred elsewhere [6] for the details.

2.2 The Three-Dimensional Point Groups

The crystallographic point groups are those groups of symmetry operations that can operate on the three-dimensional Bravais lattices so as to leave one point unmoved. They are grouped into the systems according to the lattices on which they can operate (Table 3).

Table 3
The 32 Three-Dimensional Point Groups

System	Hermann-Mauguin Notation	Schönflies Notation
Triclinic	$1, \bar{1}$	E (or C_1), S_2 (or C_i)
Monoclinic	$2, m, 2/m$	C_2, C_{1h} (or C_s), C_{2h}
Orthorhombic	$222, mm2, mmm$	D_2, C_{2v}, D_{2h}
Tetragonal	$4, \bar{4}, 4/m$ $422, 4mm$ $\bar{4}2m, 4/mmm$	C_4, S_4, C_{4h} D_4, C_{4v} D_{2d}, D_{4h}
Cubic	$23, m3, 432$ $\bar{4}3m, m3m$	T, T_h, O T_d, O_h
Trigonal	$3, \bar{3}, 32$ $3m, \bar{3}m$	C_3, S_6 (or C_{3i}), D_3 C_{3v}, D_{3d}
Hexagonal	$6, \bar{6}, 6/m$ $622, 6mm, \bar{6}m2$ $6/mmm$	C_6, C_{3h}, C_{6h} D_6, C_{6v}, D_{3h} D_{6h}

2.3 Space Groups

The space groups can be determined as the geometrically-distinct extensions of the lattices by the point groups (see Section 4).

2.3.1 One-Dimensional

There are only two one-dimensional point groups (E, C_{1h}). Since the one-dimensional lattice is simply a set of evenly spaced points along a line, there are only two possible one-dimensional space groups.

2.3.2 Two-Dimensional

There are five two-dimensional lattices (see Section 1). These can be extended by the 10 two-dimensional point groups $(E, C_2, C_{1h}, C_{2v}, C_4, C_{4v}, C_3, C_{3v}, C_6, C_{6v})$ to give 17 two-dimensional space groups. These two-dimensional space groups have application in wall-paper and textile design [7]. For example, there are only 17 geometrically-distinct types of wallpaper pattern.

2.3.3 Three-Dimensional

There are 14 three-dimensional lattices (see Section 2.1.3). These can be extended by the 32 three-dimensional point groups (Section 2.2) to give 230 three-dimensional space groups [8, 9]. These three-dimensional space groups have application in crystallographic studies using a variety of diffraction techniques [10].

2.3.4 Four-Dimensional

There are 64 four-dimensional lattices. These can be extended by the 271 four-dimensional point groups to give 4895 four-dimensional space groups [11]. The four-dimensional space groups are somewhat more abstract than the three-dimensional space groups. They have application in the magnetic properties of matter.

3. PHASE TRANSITIONS

The group-theoretic aspects of phase transitions will be discussed in detail in subsequent reports in this series. In this report we first give a summary of these properties, to establish a context for the remaining sections.

As mentioned previously, the crystalline phase of matter may exist in one or more polymorphs. The polymorph corresponding to the equilibrium structure for a given set of physical conditions is the polymorph that exhibits the lowest free energy for those conditions. If the conditions change so that a different polymorph has a lower free energy, then a phase transition must occur to restore the thermodynamic equilibrium.

Phase transitions are usually classified as being first or second order.

A first order transition is a transition characterized by a discontinuity in the free energy of the system. Such a transition requires the transfer of energy between the crystal and the surroundings at the transition point (f_t). Hence, both phases must be present at the transition point and the change of structure is gradual. The melting of a pure substance is an example of a first order transition, where the increase in free energy at the transition corresponds to the latent heat of fusion.

In a second order transition, there is a continuous structural change and no discontinuity in the free energy at the transition. The discontinuity occurs in the first derivative of the free energy with respect to the parameter that is inducing the transition. It is common practice to measure the specific heat of a substance with respect to temperature. The specific heat is the first derivative of the free energy with respect to temperature. Hence, the specific heat exhibits a discontinuity at the transition point during a second order transition. Second order transitions are often termed λ-transitions, because of the nature of the discontinuity in the specific heat (Figure 1).

Structural phase transitions were first studied by Landau, who studied order-disorder transitions in alloys [12, 13]. He showed that, for these transitions, the low symmetry phase (G^L) must be a normal subgroup of the high symmetry phase (G^H). The change in symmetry must correspond to an irreducible representation ($\tau_{k,j}$) of G^H. Hence, a vibrational or librational mode must exist in G^H that softens to induce the phase transition.

Landau showed that if the symmetrized cube of irreducible representation ($\{\tau_{k,j}\}^3$) contains the totally symmetric representation ($\tau_{\Gamma,1+}$), then the phase transition associated with $\tau_{k,j}$ must be first order. Lifshitz [14, 15] was able to show that a second order transition can occur only if the anti-symmetrized square of the representation ($[\tau_{k,j}]^2$) does not contain the representation of a polar vector ($\tau_{\Gamma,v}$).

The group-theoretic conditions for a second order (λ) transition can be expressed as follows:

1. $G^L \subset G^H$,
2. $\{\tau_{k,j}\}^3 \cap \tau_{\Gamma,1+} = 0$,
3. $[\tau_{k,j}]^2 \cap \tau_{\Gamma,v} = 0$,
4. $\tau_{k,j}$ of G^H subduces to $\tau_{\Gamma,1+}$ of G^L, and
5. $\tau_{k,j}$ corresponds to a physical tensor field.

The representational analysis of Landau and Lifshitz was supplemented by Ascher [16, 17, 18, 19] for transitions involving no change in the number of atoms per unit cell. For these transitions, Ascher was able to show that the lower symmetry group (G^L) must

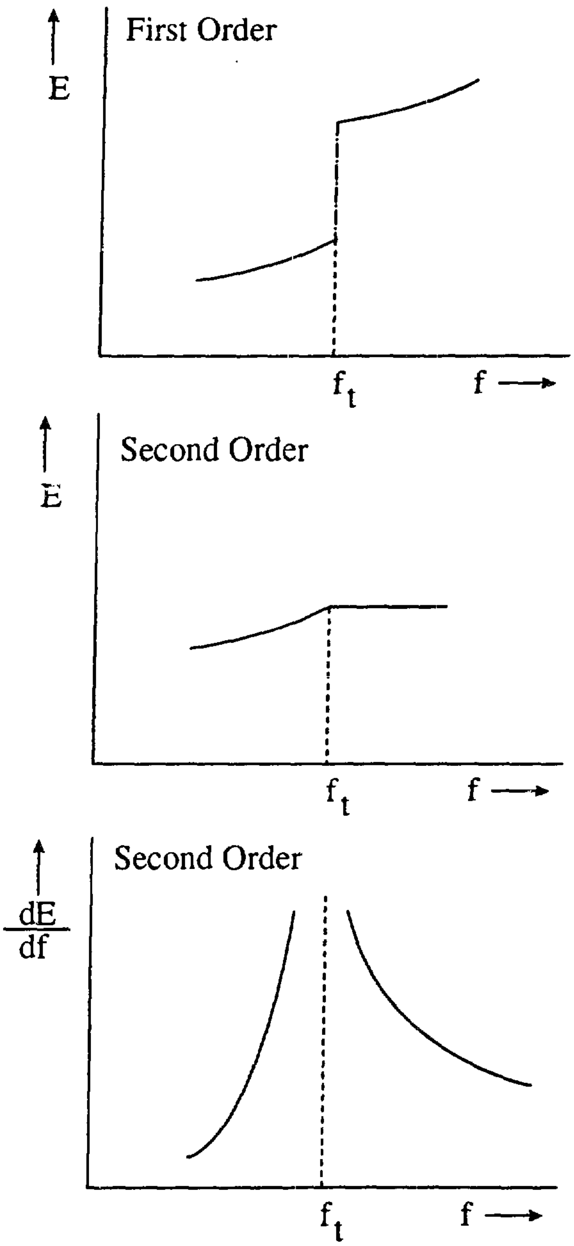

Figure 1: Thermodynamic Classification of Phase Transitions. Note the characteristic shape of dE/df for the second order (λ) transition.

be a zellengleiche subgroup[1] of the higher symmetry group (G^H). The actual subgroup (G^L) is determined by the invariance properties of the phenomenon responsible for the phase transition.

For many phase transitions (including all zellengleiche transitions), the problem of determining the appropriate irreducible representations and subgroup-supergroup relationships between the 230 space group reduces to determining the corresponding relationships between the 32 crystallographic point groups.

As will be discussed in further detail in subsequent reports in this series, group extension theory can be used to determine G^L, G^H, and $\tau_{k,j}$.

4. EXTENSIONS

The concept of extending a group was used in the nineteenth century but it was not formalized until 1926 [20, 21]. Consequently, it has not hitherto been recognized as having important applications in crystallography, except perhaps in the papers of Ascher and Janner [22, 23, 24] and in a book by Janssen [25]. Many famous problems can, however, be fruitfully formulated in terms of this concept [26]. For example, the problem of the enumeration of the 230 space groups is merely the enumeration of all the geometrically distinct extensions of the Bravais lattices (translation groups) by spatial symmetry elements. The double groups are extensions of the group containing the identity and the "2π-rotation" by the point group. The magnetic groups are the extensions of the unitary subgroup by the group containing the identity and a two-fold anti-unitary element. The representation groups [27] are extensions of Schur's multiplicator by the point group.

The structure of a point group may often be expressed in the language of group extension theory. For example, the semi-direct product groups are splitting extensions (see Section 4.5) and the direct product is included in the set of splitting extensions as the unique central splitting extension.

A group G is an extension of a group A by a group B if A is normally contained in G and the factor set G/A is isomorphic to B. That is,

$$\begin{aligned} A &\triangleleft G, \quad \text{and} \\ G/A &\cong B. \end{aligned}$$

In general, G is not unique.

The elements of A will be denoted here by Latin letters, $e, a, b, c, \ldots$, and the elements of B by Greek letters, $\epsilon, \alpha, \beta, \gamma, \ldots$. From the definition of an extension, given above, G can be decomposed into cosets of A,

$$G = g_\epsilon\{A\} + g_\alpha\{A\} + g_\beta\{A\} + \ldots,$$

[1] A zellengleiche subgroup of a space group has the same translational subgroup as the original group.

where for every coset gA of A in G we have chosen a representative, g_α, where α is the element of B associated with the coset gA in the isomorphism between G/A and B.

The product of two coset representatives $g_\alpha \cdot g_\beta$ must lie in the coset with representative $g_{\alpha\beta}$ and, hence,

$$g_\alpha \cdot g_\beta = g_{\alpha\beta} m_{\alpha,\beta}.$$

The factor system ($m_{\alpha,\beta} \in A, \forall \alpha, \beta \in B$) is not unique, and depends upon the actual choice of coset representatives. However, there are a number of relationships that restrict the value of the factor system.

Putting $\alpha = \beta = \epsilon$, we obtain

$$\begin{aligned} g_\epsilon g_\epsilon &= g_\epsilon m_{\epsilon,\epsilon}, \quad \text{and hence,} \\ g_\epsilon &= m_{\epsilon,\epsilon}. \end{aligned}$$

The transformation of A by g_α induces an automorphism in A. We shall denote the image of an element a of A under this transformation by a^α;

$$g_\alpha^{-1} a g_\alpha = a^\alpha.$$

Then

$$(a^\alpha)^\beta = (a^{\alpha\beta})^{m_{\alpha,\beta}}, \tag{1}$$

and also

$$\begin{aligned} g_\alpha g_\beta g_\gamma &= g_\alpha(g_{\beta\gamma} m_{\beta,\gamma}) = g_{\alpha\beta\gamma} m_{\alpha,\beta\gamma} m_{\beta,\gamma} = (g_{\alpha\beta} m_{\alpha,\beta}) g_\gamma \\ &= g_{\alpha\beta}(g_\gamma m^\gamma_{\alpha,\beta}) = g_{\alpha\beta\gamma} m_{\alpha\beta,\gamma} m^\gamma_{\alpha,\beta}, \end{aligned}$$

so that

$$m_{\alpha,\beta\gamma} m_{\beta,\gamma} = m_{\alpha\beta,\gamma} m^\gamma_{\alpha,\beta}. \tag{2}$$

The elements of G can be taken as $g_\alpha a$, etc., and hence the composition law for the extension is

$$g_\alpha a \cdot g_\beta b = g_{\alpha\beta} m_{\alpha,\beta} a^\beta b. \tag{3}$$

Further manipulation of the above formulae yields

$$m_{\alpha,\epsilon} = m_{\epsilon,\alpha} = m_{\epsilon,\epsilon} = e.$$

If all possible systems of automorphisms $a \rightarrow a^\alpha$ and all possible sets of factor systems are determined subject to Equations (1) and (2), then all possible extensions of A by B will have been determined. Group extensions are usually defined up to equivalence. Two groups G_1 and G_2 are said to be equivalent if there is an isomorphism between G_1 and G_2 that induces the identity automorphism on A, and also maps onto each other the cosets of A that correspond to the same element of B. If we define

$$\Phi(A)/\Phi'(A) \cong Aut(A),$$

then it can be proved that two extensions are equivalent if the same homomorphism of B into $Aut(A)$ is associated with each extension.

4.1 Extensions Of Abelian Groups

If A is an Abelian group, the problem of enumeration of the extensions is simplified somewhat. In this case, we have that since A is an Abelian normal subgroup of G the automorphisms of A induced by the coset representatives *are* independent of the actual choice of representative. Thus $Aut(A) = \Phi(A)$.

Hence, for an extension of an Abelian group A by a group B we have only to define the products $a\alpha, a \in A, \alpha \in B$, such that

$$\left.\begin{array}{rcl} (ab)\alpha & = & a\alpha \cdot b\alpha \\ a(\alpha\beta) & = & (a\alpha)\beta \\ a\epsilon & = & a \end{array}\right\} \quad (4)$$

and define the factor system $m_{\alpha,\beta}$ such that

$$m_{\alpha,\beta\gamma} m_{\beta,\gamma} = m_{\alpha\beta,\gamma} m^{\gamma}_{\alpha,\beta}. \quad (5)$$

and we will have enumerated all of the possible extensions of A by B.

4.2 Example: The Extensions Of C_4 By C_2

Let us define

$$\begin{array}{ll} C_4 = e, a, a^2, a^3 & a^4 = e \\ C_2 = \epsilon, \alpha & \alpha^2 = \epsilon. \end{array}$$

There are only two possible automorphisms of C_4:

$$\begin{array}{llllll} C_4 = & e & a & a^2 & a^3, & \text{and} \\ C_4 = & e & a^3 & a^2 & a, & \end{array}$$

hence $\Phi(C_4) = C_2$, and there are only two possible groups of operators that satisfy Equation (4).

4.2.1 $(e, a, a^2, a^3)C_2 = (e, a, a^2, a^3)$

If we consider the factor system relationship,

$$m_{\alpha,\beta\gamma} m_{\beta,\gamma} = m_{\alpha\beta,\gamma} m^{\gamma}_{\alpha,\beta},$$

it can be seen, by substitution, that no restrictions are placed on the value of m_{C_2,C_2}. Thus we have four non-equivalent extensions associated with this automorphism of A that correspond to the factor system

$$m_{\alpha,\beta} = \begin{array}{c|cc} & \epsilon & C_2 \\ \hline \epsilon & e & e \\ C_2 & e & \eta \end{array}$$

where η can take any of the values, e, a, a^2, a^3. The extensions generated by this automorphism of C_4 and these four sets of factor systems are illustrated in Figure 2.

4.2.2 $(e, a, a^2, a^3)C_2 = (e, a^3, a^2, a)$

If we again consider the factor system relationship, it can be seen that

$$m_{C_2,C_2} = (m_{C_2,C_2})C_2.$$

This equation can only be satisfied if $m_{C_2,C_2} = e$ or $m_{C_2,C_2} = a^2$. Thus we have two non-equivalent extensions associated with this automorphism of A that correspond to the factor system

$$m_{\alpha,\beta} = \begin{array}{c|cc} & \epsilon & C_2 \\ \hline \epsilon & e & e \\ C_2 & e & \eta \end{array}$$

where η can take the value e or a^2. The extensions generated by this automorphism of C_4 and these two sets of factor systems are illustrated in Figure 2.

4.3 Extensions Of Non-Abelian Groups

Baer [28] was able to show that the extensions of a non-Abelian group associated with a given homomorphism are one-to-one with the extensions of the centre (see Section 5.1) of the group associated with the same homomorphism. Thus, it is possible to obtain the extensions of a non-Abelian group, A, by generating the extensions of $Z(A)$. Hence, the extensions of all groups can be obtained from the extensions of the Abelian groups.

4.4 Central Extensions

An extension G of an Abelian group A by a group B is called *central* if A lies in the centre of G. This is equivalent to saying that the automorphisms $a \rightarrow a^\alpha$ of A corresponding to this extension are all equal to the identity. In the context of the example given in Figure 2, the groups C_{4h} and C_8 are central extensions of C_4 by C_2.

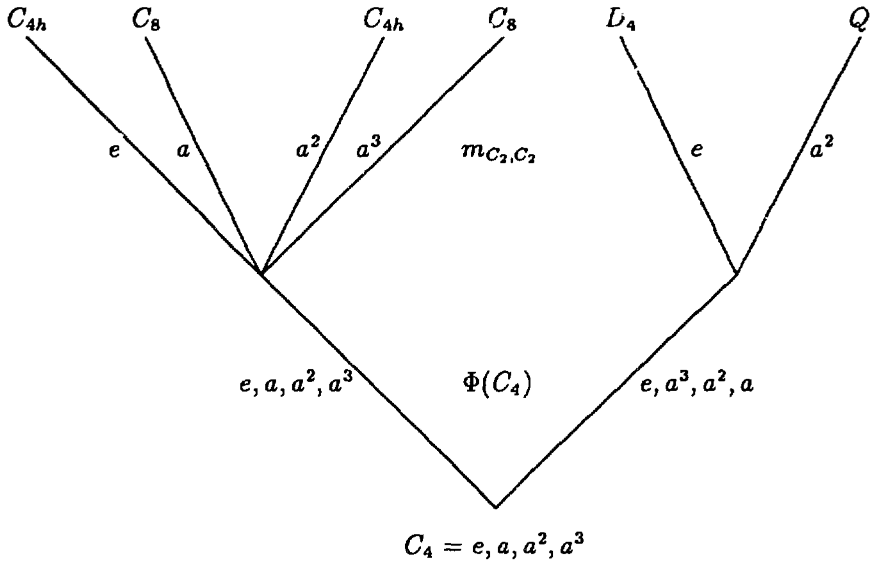

Figure 2: The Extensions of C_4 by C_2.

4.5 Splitting Extensions

Suppose G is an extension of a group A by a group B such that we can choose, in the cosets gA, representatives g_α, $\alpha \in B$, with the property

$$\begin{aligned} g_\alpha g_\beta &= g_{\alpha\beta}, \quad \text{that is} \\ m_{\alpha,\beta} &= e. \end{aligned}$$

The representatives g_α then form a subgroup (B') of G, isomorphic to B. Moreover, the subgroups A and B' completely generate G, and their intersection is E. Such an extension is said to be *splitting.* We also say that G is a *semi-direct* product of A by B'. In the context of the example given in Figure 2, the groups C_{4h} (with $m_{C_2,C_2} = e$) and D_4 are splitting extensions of C_4 by C_2. The central, splitting extension (C_{4h} with $m_{C_2,C_2} = e$) is the *direct product* of C_4 with C_2.

5. ENUMERATION OF THE AUTOMORPHISMS

In the previous sections, we have reviewed the group-theoretic properties of phase transitions and demonstrated that the problem of extending a group reduces to that of determining its automorphisms.

In this section, we derive four groups that are relevant to the determination of the automorphisms:

The Centre (Z),

The Commutator Subgroup ($\partial^1(G)$),

The Frattini φ-group, and

The Inner Automorphism Group (Φ').

The centre, commutator subgroup and Frattini φ-group are all subgroups and are straightforwardly determined. The inner automorphism group is isomorphic to the quotient of the group and its centre and, hence, is readily determined once the centre is known.

Having derived the centres, commutator subgroups, Frattini φ-groups, and the inner automorphisms groups, we use knowledge of these groups to derive the automorphisms of the crystallographic and icosahedral point groups with a consistent set of presentations. Some of the 32 crystallographic point groups do not appear in the tables, since they are isomorphic to other groups. The isomorphism relationships are given in Table 4. Some supergroups of the 32 crystallographic point groups are included where it is useful to demonstrate an *aufbau* principle. The icosahedral groups are included because some chemical compounds (e.g., $B_{12}H_{12}{}^{2-}$) are known to have icosahedral symmetry and can form crystal structures exhibiting icosahedral symmetry elements.

5.1 The Centres

The *centre* (Z) of a group, G, is that subgroup of G which contains those elements of G that commute with every element of G. The elements of Z form a group since every power or product of elements of Z must also have the commutative property and, hence, be an element of G in Z. The commutative property also implies that Z will be an Abelian group and, indeed, when G is Abelian it is its own centre. Further, Z must be a normal (or invariant) subgroup, since conjugation with respect to any elements of G will leave Z unchanged. In the context of Altmann's pole model [29, 30], the elements of Z will leave the poles of the operations of G unchanged.

For a non-Abelian point group, the matrix representing an element of Z in an irreducible representation of G will, by Schur's lemma, be a scalar multiple of the unit matrix: for an orthogonal matrix this factor will be ± 1 and, hence, the trace of the matrix will be plus or minus its dimensionality. This is the basis for an easy method of recognizing the elements of the centre by inspecting the character table of a non-Abelian group.

Alternatively, if the conjugacy class structure of a group G is known, the commutation of an element Z_i of the centre with any element G_j of G leads to $G_j^{-1} Z_i G_j = Z_i$. This implies that Z consists of all those elements of G that are in a class by themselves. The centres of the point groups are listed in Table 5.

In group extension theory the centres are important because they reduce the problem of extending a non-Abelian group to that of extending an Abelian group (see Section 4.3).

5.2 The Commutator Subgroups

The *commutator subgroup* [31] is the group generated from the products of all the commutators of the group. That is, if S is the set of all commutators of G,

$$S = \sum g_i^{-1} g_j^{-1} g_i g_j, \quad \forall\, g_i, g_j \in G,$$

then the commutator subgroup of G, $\partial^1(G)$, is the group-theoretical product of all the elements of S. That is,

$$\partial^1(G) = \prod s_i . s_j, \quad \forall\, s_i, s_j \in S.$$

The commutator subgroup is also known as the *first derived group*. The second derived group, denoted $\partial^2(G)$, is the commutator subgroup of the first derived group, i.e.,

$$\partial^2(G) = \partial^1(\partial^1(G)).$$

Table 4
Isomorphisms Between the 32 Three-Dimensional Point Groups

Group	Isomorphic Group
E	E
S_2	C_2
C_2	C_2
C_{1h}	C_2
C_{2h}	D_2
D_2	D_2
C_{2v}	D_2
D_{2h}	D_{2h}
C_4	C_4
S_4	C_4
C_{4h}	C_{4h}
D_4	D_4
C_{4v}	D_4
D_{2d}	D_4
D_{4h}	D_{4h}
T	T
T_h	T_h
O	T_d
T_d	T_d
O_h	O_h
C_3	C_3
S_6	C_6
D_3	D_3
C_{3v}	D_3
D_{3d}	C_{6h}
C_6	C_6
C_{3h}	C_6
C_{6h}	C_{6h}
D_6	D_6
C_{6v}	D_6
D_{3h}	D_6
D_{6h}	D_{6h}

The major use of the commutator subgroup is to determine the solvability of a group. The usual definition of a solvable group is a group that has a finite subnormal series with last term identity and that has an Abelian series of factor groups. That is,

$$E = G_n \lhd \ldots \lhd G_2 \lhd G_1 \lhd G_0 = G, \quad \text{with } G_i/G_{i+1} \text{ Abelian.}$$

This cumbersome definition can be replaced by a definition involving commutator subgroups that is much easier to calculate: a solvable group is one that has a derived chain that terminates on the identity. That is, G is solvable if

$$E = \partial^n(G) \subset \ldots \subset \partial^2(G) \subset \partial^1(G) \subset \partial^0(G) = G.$$

An Abelian group has $\partial^1(G) = E$. A *perfect* group has $\partial^1(G) = G$ and is *not* solvable. The commutator subgroups of the point groups are given in Table 5. This table shows that the point groups of crystallographic importance are solvable with the exception of the icosahedral groups. The icosahedral groups (I and I_h) are not solvable since $\partial^1(I_h) = I$, and I is a perfect group.

5.3 The Frattini φ-Groups

The *Frattini φ-group* is defined [32] as the intersection of all the maximal subgroups of the group under investigation.

The Frattini φ-group is important in the presentation of a group. The φ-group is the set of non-generators of the group. That is, if a set of generators is devised for a group that contains an element of the φ-group, then the element of the φ-group can always be removed from the set of generators and the set will still completely generate the group. The Frattini φ-groups of the point groups are given in Table 5.

5.4 The Inner Automorphism Groups

The *inner automorphism group* (Φ') of a group G is defined as the group of all automorphisms of G that can be generated by conjugating elements. Conjugation with the element G_j maps the element G_i onto $G_j^{-1}G_iG_j$. When all the elements G_i of G are considered, the conjugation is an automorphism of the group G. In general, some of these automorphisms will be the same and we must find out how to choose a set of different automorphisms that have the group property. The clue to this is that whenever an element G_j belongs to the centre of G, the automorphism will be the identity automorphism. Since the centre is an invariant subgroup, we can define a factor group G/Z and, hence, classify the elements of G into cosets. The elements of a given coset will produce the same automorphism of G and, hence, the factor group G/Z satisfies the requirements for Φ'. It should be stressed that while G/Z is always isomorphic to a subgroup of G, the inner automorphism group itself is *not* a subgroup of G. To illustrate this let us consider the case when G is the point group C_{4v}. The centre Z is C_2 and G/Z is isomorphic to C_{2v}, which may be presented as $P^2 = Q^2 = E, PQ = QP$. The action of the generators (P and Q) of Φ' on the generators (C_4 and σ_v^{xz}) of C_{4v} may be expressed as $\hat{P}C_4 = C_4$, $\hat{P}\sigma_v^{xz} = C_4^2\sigma_v^{xz} = \sigma_v^{yz}$, $\hat{Q}C_4 = C_4^3$, $\hat{Q}\sigma_v^{xz} = \sigma_v^{xz}$. It can thus be verified that P and Q cannot be identified with any of the elements of C_{4v}. Note that saying the automorphism P is produced by *conjugation* with one of the four-fold elements of C_{4v} is *not* the same as saying that P is C_4 or C_4^3: P is a *two-fold* element of Φ'. The inner automorphism groups of the point groups are tabulated in Table 5, and the effects of their generators on the point groups are included in Tables 6–10.

Table 5

The Centres, Commutator Subgroups, Frattini φ-Groups, and Inner Automorphism Groups of the Point Groups

Group	Centre	Commutator Subgroup	Frattini φ-Group	Inner Automorphism Group
C_2	C_2	E	C_2	E
C_3	C_3	E	C_3	E
C_4	C_4	E	C_2	E
C_5	C_5	E	C_5	E
C_6	C_6	E	E	E
D_2	D_2	E	E	E
D_3	E	C_3	E	D_3
D_4	C_2	C_2	E	D_2
D_5	E	C_5	E	D_5
D_6	C_2	C_3	E	D_3
D_{2h}	D_{2h}	E	E	E
D_{4h}	C_{2h}	C_2	E	D_2
D_{5h}	C_{1h}	C_5	E	E
D_{6h}	C_{2h}	C_3	E	D_3
C_{4h}	C_{4h}	E	C_2	E
C_{5h}	C_{5h}	E	E	E
C_{6h}	C_{6h}	E	E	E
T	E	D_2	E	T
T_d	E	T	E	T_d
T_h	S_2	D_2	E	T
O_h	S_2	T	E	O
I	E	I	E	I
I_h	S_2	I	E	I

5.5 The Outer Automorphism Groups

The *outer automorphism group* (Φ) is the group of all possible automorphisms of G. The inner automorphism group is a subgroup of the outer automorphism group. There is no little formula like G/Z or conjugation process to determine Φ. The determination of Φ is considerably more difficult and more abstract than the determination of the inner automorphism group. Nevertheless, the outer automorphism group is required if one wishes to study all possible extensions of a given group. Such exhaustive studies are not only necessary when one attempts an enumeration problem, but also when one is looking for an extension with a particular property.

First, one may dispense with the complete groups (i.e., those that are isomorphic with their automorphism groups). For this to be the case, the centre Z must contain the identity only, but this is not a sufficient condition. Hölder [33] was able to show that the full permutation, or "symmetric", groups, $P_n\,(3 \leq n \neq 6)$ were complete and hence since the point groups C_{3v} and D_3 are isomorphic to P_3, and T_d and O are isomorphic to P_4, the outer automorphism groups are known for these groups. The actions of the generators of the automorphism groups on these point groups will be elucidated in the subsequent sections.

Hölder was also able to find the outer automorphism groups for the alternating groups (i.e., the groups of even permutations), $A_n\,(5 \leq n \neq 6)$. He showed that these were isomorphic to the corresponding full permutation group. Since the icosahedral rotation group, I, is isomorphic to A_5, its outer automorphism group is isomorphic to P_5.

The outer automorphism groups of the remaining point groups can be deduced by an ***aufbau*** process in which the groups are presented in terms of a complete set of independent generators. The single-generator, or cyclic, groups must, therefore, be considered first.

5.5.1 Cyclic Groups, C_n and S_n

The cyclic group of order n can be generated by any one of its n-fold elements. If the n elements are written $C_n^i\,(1 \leq i \leq n-1)$, then the order of C_n^i is the highest common factor (hcf) of n and i. The number of n-fold elements is thus $\sum_{i=1}^{n-1} \delta_{\{\mathrm{hcf}(i,n),1\}}$, where δ is the Kronecker delta that takes the value $+1$ if $\mathrm{hcf}(i,n) = 1$ and zero if $\mathrm{hcf}(i,n) \neq 1$. This function of the number n is known as Euler's ϕ-function [34], although it was Gauss [35] rather than Euler who used the letter ϕ: Euler used πn in his original work. The order of the outer automorphism group is precisely $\phi(n)$. If $\phi(n)$ is prime, then $\Phi(C_n) = C_{\phi(n)}$.

If $\phi(n)$ is composite, rather than prime, $\Phi(C_n)$ is determined using a formulation derived by Hilton [36]. The subset of the numbers $i\,(1 \leq i \leq n-1)$ such that $\mathrm{hcf}(i,n) = 1$ form an Abelian group under multiplication modulo n. This group is known as the multiplicative group of units of the ring of numbers $Z_n = \{0, 1, 2, \ldots, n-1\}$ and is denoted by $U(Z_n)$.

Hilton showed that $\Phi(C_n) \cong U(Z_n)$ if $\phi(n)$ is composite.

A useful property of Euler's ϕ-function is that when the integers n_1 and n_2 are relatively prime (i.e., $\text{hcf}(n_1, n_2) = 1$), $\phi(n_1 n_2) = \phi(n_1)\phi(n_2)$. Consequently, the structure of the automorphism group of $C_{n_1 n_2}$ will be the direct product of the automorphism groups of C_{n_1} and C_{n_2}.

5.5.2 Two-Generator Groups

Those point groups that can be specified by two generators are either direct products (e.g., C_{2nh}) or semi-direct products (e.g., $C_{nv} \cong D_n \cong D_{\frac{n}{2}d}$ (n even)). Of these, $C_{2v} \cong D_2 \cong C_{2h}$ is a special case.

5.5.2.1 Dihedral Groups, D_n and C_{nv}

The dihedral groups are defined abstractly by two generators, A and B, such that $A^n = B^2 = E$ and $BA = A^{n-1}B$. The choice of the n-fold generator A is completely determined by the automorphisms of the cyclic group C_n. The two-fold generator B must be one of the n elements $A^pB\,(0 \leq p \leq n-1)$. The choice of B is therefore n-fold and, since it may be chosen freely, is defined by a cyclic permutation group isomorphic to C_n. To find the structure of $\Phi(D_n)$ we need to study the effects of its generators on the elements of D_n. We cannot assume that, because the choice of A and B is free, the group $\Phi(D_n)$ must have the direct product structure $\Phi(C_n) \times C_n$ as the following derivation shows.

Let $\Phi(D_n)$ be presented as an extension of $\Phi(C_n)$ by the generator P such that $P^n = E$ and let Q be any element of $\Phi(C_n)$. Then, the structure of $\Phi(D_n)$ is known if we can express all elements of the type QP in terms of standard elements P^jQ^k. To do this the effect of QP on the general element A^lB of D_n must be studied. By definition,

$$\hat{P}A = A, \quad \hat{P}B = A^pB \qquad (0 \leq p \leq n-1), \quad \text{and}$$
$$\hat{Q}A = A^q\,(\text{hcf}(q,n) = 1), \quad \hat{Q}B = B.$$

Hence,

$$\hat{Q}\hat{P}(A^lB) = \hat{Q}(A^{l+p}B) = A^{lq+pq}B, \quad \text{and}$$
$$\hat{P}^j\hat{Q}^k(A^lB) = \hat{P}^j(A^{lqk}B) = A^{lqk+pj}B.$$

QP can therefore be identified with the element P^jQ^k of $\Phi(D_n)$ if $j = q$ and $k = 1$. The relationship between a generator Q of $\Phi(C_n)$ and P is therefore such that $QP = P^qQ$. Since $\Phi(C_n)$ always contains the inverse automorphism when $n > 2$, it must always contain a subgroup isomorphic to D_n. When $n = 3$, 4 or 6, there are no other generators in $\Phi(C_n)$ and hence $\Phi(D_n) \cong D_n$ in these cases. Although $\Phi(D_n) \cong D_n$ for $n = 4$ and 6, it is not the inner automorphism group, since it cannot be generated by the conjugation process from elements of D_n. In these cases the inner automorphism group is a halving subgroup of $\Phi(D_n)$. The order of $\Phi(D_n)$ is $n\phi(n)$.

5.5.2.2 The C_{nh} Groups

The C_{nh} groups are direct product groups and hence can be defined abstractly by two independent generators A and B such that $A^n = B^2 = E$ and $BA = AB$. When n is odd, the C_{nh} group is cyclic and its automorphism group is isomorphic to the group $\Phi(C_{2n})$ determined above. When n is even, there is a difference between the C_{4nh} and $C_{(4n+2)h}$ families, since these respectively contain $2\phi(4n)$ $4n$-fold and $3\phi(4n+2)$ $(4n+2)$-fold elements, any of which could be chosen as the generator A.

The outer automorphism groups of the $C_{(4n+2)h}$ $(n \geq 1)$ family may be considered as generated by the generators of the group $\Phi(C_{4n+2})$. Operator Q has the effects $\hat{Q}A = A^q$ $(\mathrm{hcf}(q, 4n+2) = 1)$ and $\hat{Q}B = B$. Operator P has the effects $\hat{P}A = A$, $\hat{P}B = A^{2n+1}B$. Operator R has the effects $\hat{R}A = AB$ and $\hat{R}B = A^{2n+1}$. The operators P and R are such that $P^2 = R^3 = E$ and $RP = PR^2$, and hence form a group of order six isomorphic to the dihedral group D_3. P and R commute with all operators Q and hence $\Phi(C_{4n+2})$ is a factor in a direct product structure. $\Phi(C_{(4n+2)h})$ is therefore isomorphic to $D_3 \times \Phi(C_{4n+2})$ and is of order $6\phi(4n+2)$. In the case of the crystallographic point group C_{6h}, the outer automorphism group will accordingly be isomorphic to $D_3 \times C_2$ (i.e., D_6).

The outer automorphism groups of the C_{4nh} family will be generated in a similar way. However, the operator R, which has the effects $\hat{R}A = AB$ and $\hat{R}B = A^{2n}B$, is such that R^2 is one of the operators of $\Phi(C_{4n})$, since $\hat{R}^2A = A^{2n+1}$ and $\hat{R}^2B = B$. If, therefore, we consider only those operators Q which correspond to indices $q < 2n$ in the definition $\hat{Q}A = A^q$ $(\mathrm{hcf}(q, 4n) = 1)$ and $\hat{Q}B = B$, the operators Q for which $q > 2n$ can always be expressed as R^2 times a Q for which $q < 2n$. This restricted class of operators Q generates the factor group $\Phi(C_{4n})/\{E, R^2\}$ where $\{E, R^2\}$ is a group of two elements isomorphic to C_2. Since P (which is defined to have the effects $\hat{P}A = A$ and $\hat{P}B = A^{2n}B$) and R both commute with the operations of the factor group, $\Phi(C_{4n})/\{E, R^2\}$ is a factor in a direct product structure. The operators P and R are such that $P^2 = R^4 = E$ and $RP = PR^3$ and, hence, form a group of order 8 isomorphic to the dihedral group D_4. The structure of $\Phi(C_{4nh})$ is then isomorphic to $D_4 \times \{\Phi(C_{4n})/C_2\}$ and is a group of order $4\phi(4n)$. In the case of the crystallographic group C_{4h}, the automorphism group $\Phi(C_{4h})$ is isomorphic to D_4.

5.5.2.3 The D_{nd} Groups

The D_{nd} groups are isomorphic to D_{2n} when n is even and to C_{2nh} when n is odd. Their outer automorphism groups are, therefore, isomorphic to the outer automorphism groups of these groups, which have been determined above.

5.5.2.4 Klein's *Vierergruppe* (C_{2v}, D_2, or C_{2h})

The determination of the outer automorphism group of this Abelian group was presented by Hölder [33]. Its elements may be written in terms of two generators as $\{E, A, B, AB\}$. There is a choice of three elements for the generator A which, once chosen, leaves a choice of two for B. The third two-fold element is then the product of the two generators. The order of $\Phi(C_{2v})$ is $3 \times 2 = 6$ and its group may be presented as

$$\hat{P}A = A \quad \hat{P}B = AB$$
$$\hat{Q}A = AB \quad \hat{Q}B = A$$

where $P^2 = Q^3 = E$ and $QP = PQ^2$. $\Phi(C_{2v})$ is, therefore, isomorphic to the dihedral group D_3.

5.5.3 The D_{nh} Groups

5.5.3.1 The $D_{(2n+1)h}$ Groups

The $D_{(2n+1)h}$ groups are isomorphic to the D_{4n+2} dihedral groups. Hence, the automorphisms of the $D_{(2n+1)h}$ groups can be calculated by the method given in Section 5.5.2.1.

5.5.3.2 The D_{2nh} ($n > 1$) Groups

These groups, which are defined by $A^{2n} = B^2 = C^2 = E$, $BA = A^{2n-1}B$, $CA = AC$, and $BC = CB$, may be conveniently separated into a C_{2nh} part and a dihedral part.

$$D_{2nh} = \{C_{2nh}\} + \{nC_2' + nC_2'' + n\sigma_v + n\sigma_d\}.$$

Now, due to the order and class structure of these groups, it is not possible for an automorphism to map any of the C_{2nh} elements onto the dihedral part elements. Therefore, the generators A and C of D_{2nh} are completely determined by an automorphism of C_{2nh}. It only remains to make a choice for the generating element B.

From the point of view of acting as a generator, all of the $4n$ dihedral elements are equivalent. Hence, the choice for the generating element B ranges over all of the $4n$ dihedral elements. The automorphisms generated from B form the Abelian group C_{2nh}, which is normal in $\Phi(D_{2nh})$. Hence, we obtain a semi-direct product for the isomorphism group of D_{2nh}

$$\Phi(D_{2nh}) \cong C_{2nh} \wedge \Phi(C_{2nh}).$$

The automorphisms of the C_{2nh} groups are divided into two families (see Section 5.5.2.2). Hence, we obtain for $n > 1$,

$$\begin{aligned}\Phi(D_{4nh}) &\cong C_{4nh} \wedge \{D_4 \times \{\Phi(C_{4n})/C_2\}\},\\ &\cong C_{4nh} \wedge \{D_4 \times \{U(Z_{4n})/C_2\}\},\end{aligned}$$

and

$$\begin{aligned}\Phi(D_{(4n+2)h}) &\cong C_{(4n+2)h} \wedge \{D_3 \times \Phi(C_{4n+2})\},\\ &\cong C_{(4n+2)h} \wedge \{D_3 \times U(Z_{4n+2})\}.\end{aligned}$$

5.5.3.3 The D_{2h} Group

The D_{2h} group is defined by $A^2 = B^2 = C^2 = E$, with $AB = BA$, $BC = CB$, and $AC = CA$. Generator A is of the same order (i.e., 2) as the generators B and C. This prevents the separation into a C_{2nh} subgroup and a dihedral part and, hence, $\Phi(D_{2h})$ cannot be determined by the method given in Section 5.5.3.2.

The choice of generator A ranges over any of the seven two-fold elements. Similarly, the generator B may range over any of the six remaining two-fold elements. These two generators, A and B, generate the dihedral group D_2. The choice for generating element C is thus restricted to any of the four two-fold elements that are not contained in the above dihedral group. Hence, the automorphisms of the group D_{2h} form a group of order 168.

$$o(\Phi(D_{2h})) = 7 \times 6 \times 4 = 168.$$

This group, whose actions are given in Table 6, is isomorphic to Klein's simple group [37].

5.5.4 Cubic Groups

5.5.4.1 The T_d Group

The T_d group is fundamental to the construction of the automorphisms of the cubic groups. The T_d group is isomorphic to the permutation group P_4. As has been mentioned previously, P_4 is complete, therefore

$$\Phi(T_d) \cong T_d.$$

5.5.4.2 The T Group

The group T_d can be decomposed into its subgroup, T, and the remaining part $\{T_d - T\}$:

$$\begin{array}{llcl} T_d = & \{E + 4C_3 + 4C_3^2 + 3C_2\} & + & \{6S_4 + 6\sigma_d\} \\ & A^3 = B^2 = C^2 = E & & D^2 = E \\ & BA = AC & & DA = A^2CD \\ & CB = BC & & DB = BD \\ & CA = ABC & & DC = BCD. \end{array}$$

The generating relations ensure that, given a presentation of the group T, there is only one possible choice for the generator D. Hence, every automorphism of T_d is induced by a single automorphism of the group T. The automorphisms of the groups T and T_d must be one-to-one. Therefore,

$$\Phi(T) \cong \Phi(T_d) \cong T_d.$$

5.5.4.3 The T_h Group

The group T_h can also be split into the subgroup T and the part $\{T_h - T\}$:

$$\begin{array}{llcl} T_h = & \{E + 4C_3 + 4C_3^2 + 3C_2\} & + & \{S_2 + 4S_6 + 4S_6^2 + 3\sigma_d\} \\ & A^3 = B^2 = C^2 = E & & D^2 = E \\ & BA = AC & & DA = AD \\ & CB = BC & & DB = BD \\ & CA = ABC & & DC = CD. \end{array}$$

As was the case for the T_d group, for a specific presentation of the group T, the generating relations ensure that there is only one possible choice for the generating element D. Therefore,

$$\Phi(T_h) \cong \Phi(T) \cong \Phi(T_d) \cong T_d.$$

5.5.4.4 The O_h Group

The cubic group O_h can be conveniently decomposed into its cubic subgroup O and the remaining part $\{O_h - O\}$:

$$\begin{array}{llcl} O_h = & \{E + 8C_3 + 6C_2 + 6C_4 + 3C_2\} & + & \{S_2 + 6S_4 + 8S_6 + 3\sigma_h + 6\sigma_d\} \\ & \text{The Subgroup } O & & \end{array}$$

The group O is isomorphic to the group T_d, and hence is complete:

$$\Phi(O) \cong \Phi(T_d) \cong T_d \cong O.$$

In addition to the automorphisms induced by those of the group O, there is the class of automorphisms generated by the mapping:

$$\begin{array}{rcl} 6C_2^i & \rightarrow & 6\sigma_d^i \\ 6C_4^i & \rightarrow & 6S_4^i \\ 6S_4^i & \rightarrow & 6C_4^i \\ 6\sigma_d^i & \rightarrow & 6C_2^i. \end{array}$$

This two-fold automorphism commutes with all of the automorphisms generated by the automorphisms of O, and hence we obtain

$$\Phi(O_h) \cong \Phi(O) \times C_2 \cong O \times C_2 \cong O_h.$$

5.5.5 Icosahedral Groups

5.5.5.1 The I Group

The automorphisms of the group I can be deduced by considering the class structure of the group:

$$I = \{12C_5\} + \{12C_5^2\} + \{20C_3\} + \{15C_2\}.$$

It is well known that the group of inner automorphisms of I is isomorphic to I, since

$$\Phi'(I) \cong I/Z(I) \cong I/\{E\} \cong I.$$

Now, because of the class structure of I, the only two classes that can be interchanged by an automorphism are $\{12C_5\}$ and $\{12C_5^2\}$. These classes cannot be interchanged by an inner automorphism. Hence, if we produce a mapping $\{12C_5\} \leftrightarrow \{12C_5\}$ we are able to produce a complete set of automorphisms. The automorphism so produced does not commute with any of the inner automorphisms of the group, because of the class structure. Hence, the group of automorphisms is isomorphic to the permutation group P_5; i.e.,

$$\Phi(I) \cong P_5.$$

5.5.5.2 The I_h Group

The group I_5 is the direct product of the group I with the group S_2. Due to the structure of the group it is possible to choose the additional generator (S_2) in only one way. In addition, no class of $\{I_h - I\}$ may be permuted by an automorphism with any class of I, due to the order structure of the group. Hence, every automorphism of I_h is induced by a single automorphism of I,

$$\Phi(I_h) \cong \Phi(I) \cong P_5.$$

Table 6
The Automorphisms of the Cyclic Groups

Group	Presentation	Φ'	Φ		
			Group	Presentation	Action
C_2	$A^2 = E$	E	E	E	
C_3	$A^3 = E$	E	C_2	$P^2 = E$	$\hat{P}A = A^2$
C_4	$A^4 = E$	E	C_2	$P^2 = E$	$\hat{P}A = A^3$
C_5	$A^5 = E$	E	C_4	$P^4 = E$	$\hat{P}A = A^2$
C_6	$A^6 = E$	E	C_2	$P^2 = E$	$\hat{P}A = A^5$
C_{10}	$A^{10} = E$	E	C_4	$P^4 = E$	$\hat{P}A = A^3$

Table 7
The Automorphisms of the Two-Generator Point Groups

Group	Presentation	Φ'	Φ		
			Group	Presentation	Action
D_2	$A^2 = B^2 = E$ $AB = BA$	E	D_3	$P^3 = Q^2 = E$ $QP = P^2Q$	$\hat{P}A = B$ $\hat{P}B = AB$ $\hat{Q}A = B$ $\hat{Q}B = A$
D_3	$A^3 = B^2 = E$ $BA = A^2B$	D_3	D_3	$P^3 = Q^2 = E$ $QP = P^2Q$	$\hat{P}A = A$ $\hat{P}B = A^2B$ $\hat{Q}A = A^2$ $\hat{Q}B = A^2B$
D_4	$A^4 = B^2 = E$ $BA = A^3B$	D_2	D_4	$P^4 = Q^2 = E$ $QP = P^3Q$	$\hat{P}A = A$ $\hat{P}B = AB$ $\hat{Q}A = A^3$ $\hat{Q}B = B$
D_5	$A^5 = B^2 = E$ $BA = A^4B$	D_5	$C_5 \wedge C_4$	$P^5 = Q^4 = E$ $QP = P^3Q$	$\hat{P}A = A$ $\hat{P}B = A^2B$ $\hat{Q}A = A^2$ $\hat{Q}B = B$
D_6	$A^6 = B^2 = E$ $BA = A^5B$	D_3	D_6	$P^6 = Q^2 = E$ $QP = P^5Q$	$\hat{P}A = A$ $\hat{P}B = AB$ $\hat{Q}A = A^5$ $\hat{Q}B = B$

Continued...

Table 7
The Automorphisms of the Two-Generator Point Groups (Concluded)

Group	Presentation	Φ'	Φ		
			Group	Presentation	Action
D_8	$A^8 = B^2 = E$ $BA = A^7B$	D_4	$C_8 \wedge D_2$	$P^8 = Q^2 = R^2 = E$ $QP = P^7Q$ $RP = P^3R$ $QR = RQ$	$\hat{P}A = A$ $\hat{P}B = AB$ $\hat{Q}A = A^7$ $\hat{Q}B = B$ $\hat{R}A = A^3$ $\hat{R}B = B$
D_{10}	$A^{10} = B^2 = E$ $BA = A^9B$	D_5	$C_{10} \wedge C_4$	$P^{10} = Q^4 = E$ $QP = P^7Q$	$\hat{P}A = A$ $\hat{P}B = AB$ $\hat{Q}A = A^3$ $\hat{Q}B = B$
D_{12}	$A^{12} = B^2 = E$ $BA = A^{11}B$	D_6	$C_{12} \wedge D_2$	$P^{12} = Q^2 = R^2 = E$ $QP = P^{11}Q$ $RP = P^5R$ $QR = RQ$	$\hat{P}A = A$ $\hat{P}B = AB$ $\hat{Q}A = A^{11}$ $\hat{Q}B = B$ $\hat{R}A = A^5$ $\hat{R}B = B$
C_{4h}	$A^4 = B^2 = E$ $BA = AB$	E	D_4	$P^4 = Q^2 = E$ $QP = P^3Q$	$\hat{P}A = AB$ $\hat{P}B = A^2B$ $\hat{Q}A = A$ $\hat{Q}B = A^2B$
C_{6h}	$A^6 = B^2 = E$ $BA = AB$	E	D_6	$P^6 = Q^2 = E$ $QP = P^3Q$	$\hat{P}A = A^2B$ $\hat{P}B = A^3B$ $\hat{Q}A = A$ $\hat{Q}B = A^3B$

Table 8
The Automorphisms of the D_{2nh} Groups

Group	Presentation	Φ'	Φ		
			Group	Presentation	Action
D_{2h}	$A^2 = B^2 = C^2 = E$ $AB = BA$ $CA = AC$ $CB = BC$	E	Klein's Simple Group of Order 168	$P^4 = Q^7 = (PQ)^2 =$ $(P^{-1}Q)^3 = E$	$\hat{P}A = A$ $\hat{P}B = C$ $\hat{P}C = AB$ $\hat{Q}A = B$ $\hat{Q}B = AC$ $\hat{Q}C = A$
D_{4h}	$A^4 = B^2 = C^2 = E$ $BA = A^3B$ $CA = AC$ $CB = BC$	D_2	$C_{4h} \wedge D_4$	$P^4 = Q^2 = R^4 =$ $S^2 = E$ $QP = P^3Q$ $SR = RS$ $PR = RSP$ $PS = R^2SP$ $QR = RQ$ $QS = R^2SQ$	$\hat{P}A = AC$ $\hat{P}B = B$ $\hat{P}C = A^2C$ $\hat{Q}A = A$ $\hat{Q}B = B$ $\hat{Q}C = A^2C$ $\hat{R}A = A$ $\hat{R}B = AB$ $\hat{R}C = C$ $\hat{S}A = A$ $\hat{S}B = BC$ $\hat{S}C = C$
D_{6h}	$A^6 = B^2 = C^2 = E$ $BA = A^5B$ $CA = AC$ $CB = BC$	D_3	$C_{6h} \wedge D_6$	$P^6 = Q^2 = R^6 =$ $S^2 = E$ $QP = P^5Q$ $SR = RS$ $PR = R^5SP$ $QR = RQ$ $PS = R^3P$ $QS = R^3SQ$	$\hat{P}A = A^5C$ $\hat{P}B = B$ $\hat{P}C = A^3$ $\hat{Q}A = A$ $\hat{Q}B = B$ $\hat{Q}C = A^3C$ $\hat{R}A = A$ $\hat{R}B = AB$ $\hat{R}C = C$ $\hat{S}A = A$ $\hat{S}B = BC$ $\hat{S}C = C$

Table 9
The Automorphisms of the Cubic Groups

Group	Presentation	Φ'	Φ		
			Group	Presentation	Action
T	$A^3 = B^2 = C^2 = E$ $BA = AC$ $BC = CB$ $CA = ABC$	T	T_d	$P^3 = Q^2 = R^2 =$ $S^2 = E$ $QP = PR$ $RQ = QR$ $RP = PQR$ $SP = P^2RS$ $SQ = QS$ $SR = QRS$	$\hat{P}A = A$ $\hat{P}B = BC$ $\hat{P}C = B$ $\hat{Q}A = CA$ $\hat{Q}B = B$ $\hat{Q}C = C$ $\hat{R}A = BCA$ $\hat{R}B = B$ $\hat{R}C = C$ $\hat{S}A = A^2BC$ $\hat{S}B = B$ $\hat{S}C = BC$
T_d	$A^3 = B^2 = C^2 = D^2 = E$ $BA = AC$ $CA = ABC$ $CB = BC$ $DA = A^2CD$ $DB = BD$ $DC = BCD$	T_d	T_d	$P^3 = Q^2 = R^2 =$ $S^2 = E$ $QP = PR$ $RP = PQR$ $RQ = QR$ $SP = P^2RS$ $SQ = QS$ $SR = QRS$	$\hat{P}A = A$ $\hat{P}B = BC$ $\hat{P}C = B$ $\hat{P}D = A^2BCD$ $\hat{Q}A = ABC$ $\hat{Q}B = B$ $\hat{Q}C = C$ $\hat{Q}D = D$ $\hat{R}A = AB$ $\hat{R}B = B$ $\hat{R}C = C$ $\hat{R}D = BD$ $\hat{S}A = A^2BC$ $\hat{S}B = B$ $\hat{S}C = BC$ $\hat{S}D = BD$

Continued...

Table 9
The Automorphisms of the Cubic Groups (Concluded)

Group	Presentation	Φ'	Φ		
			Group	Presentation	Action
T_h	$A^6 = B^2 = C^2 = E$ $BA = ABC$ $CA = AB$ $CB = BC$	T	T_d	$P^3 = Q^2 = R^2 = S^2 = E$ $QP = PR$ $RP = PQR$ $RQ = QR$ $SP = P^2RS$ $SQ = QS$ $SR = QRS$	$\hat{P}A = A$ $\hat{P}B = BC$ $\hat{P}C = B$ $\hat{Q}A = A^2BC$ $\hat{Q}B = B$ $\hat{Q}C = C$ $\hat{R}A = ABC$ $\hat{R}B = B$ $\hat{R}C = C$ $\hat{S}A = A^5BC$ $\hat{S}B = B$ $\hat{S}C = BC$
O_h	$A^6 = B^2 = C^2 = D^2 = E$ $BA = AC$ $BA^3 = A^3B$ $CA = A^4BC$ $BC = CB$ $DA = A^2BD$ $DB = CD$ $DC = BD$	O	O_h	$P^6 = Q^2 = R^2 = S^2 = E$ $QP = PR$ $QP^3 = P^3Q$ $RP = P^4QR$ $RQ = QR$ $SP = P^2QS$	$\hat{P}A = A$ $\hat{P}B = C$ $\hat{P}C = A^3BC$ $\hat{P}D = A^4BD$ $\hat{Q}A = ABC$ $\hat{Q}B = B$ $\hat{Q}C = C$ $\hat{Q}D = A^3BCD$ $\hat{R}A = A^4B$ $\hat{R}B = B$ $\hat{R}C = C$ $\hat{R}D = A^3BCD$ $\hat{S}A = A^2B$ $\hat{S}B = C$ $\hat{S}C = B$ $\hat{S}D = D$

Table 10
The Automorphisms of the Icosahedral Groups

Group	Presentation	Φ'	Φ		
			Group	Presentation	Action
I	$A^5 = B^3 = C^2 =$	I	P_5	$P^5 = Q^3 = R^2 =$	$\hat{P}A = A$
	$D^2 = E$			$S^2 = T^2 = E$	$\hat{P}B = A^3B^2$
	$BA = A^4B^2$			$QP = P^4Q^2$	$\hat{P}C = AB$
	$CA = A^2B$			$RP = P^2Q$	$\hat{P}D = A^4D$
	$DA = A^4D$			$SP = P^4S$	$\hat{Q}A = A^3C$
	$BD = CB$			$QS = RQ$	$\hat{Q}B = B$
	$DC = CD$			$SR = RS$	$\hat{Q}C = D$
	$DB = CB^2$			$SQ = RQ^2$	$\hat{Q}D = CD$
				$TP = P^3SQ^2T$	$\hat{R}A = A^2BC$
				$TQ = QT$	$\hat{R}B = BCD$
				$TR = PQ^2RST$	$\hat{R}C = C$
				$TS = SQP^2T$	$\hat{R}D = D$
					$\hat{S}A = A^4$
					$\hat{S}B = BC$
					$\hat{S}C = C$
					$\hat{S}D = D$
					$\hat{T}A = B^2AD$
					$\hat{T}B = B$
					$\hat{T}C = ACB^2$
					$\hat{T}D = A^3B^2D$

Continued...

Table 10
The Automorphisms of the Icosahedral Groups (Concluded)

Group	Presentation	Φ'	Φ		
			Group	Presentation	Action
I_h	$A^5 = B^3 = C^2 =$	I	P_5	$P^5 = Q^3 = R^2 =$	$\hat{P}A = A$
	$D^2 = I^2 = E$			$S^2 = T^2 = E$	$\hat{P}B = A^3B^2$
	$BA = A^4B^2$			$QP = P^4Q^2$	$\hat{P}C = AB$
	$CA = A^2B$			$RP = P^2Q$	$\hat{P}D = A^4D$
	$DA = A^4D$			$SP = P^4S$	$\hat{Q}A = A^3C$
	$BD = CB$			$QS = RQ$	$\hat{Q}B = B$
	$DC = CD$			$SR = RS$	$\hat{Q}C = D$
	$DB = CB^2$			$SQ = RQ^2$	$\hat{Q}D = CD$
	$AI = IA$			$TP = P^3SQ^2T$	$\hat{R}A = A^2BC$
	$BI = IB$			$TQ = QT$	$\hat{R}B = BCD$
	$CI = IC$			$TR = PQ^2RST$	$\hat{R}C = C$
	$DI = ID$			$TS = SQP^2T$	$\hat{R}D = D$
					$\hat{S}A = A^4$
					$\hat{S}B = BC$
					$\hat{S}C = C$
					$\hat{S}D = D$
					$\hat{T}A = B^2AD$
					$\hat{T}B = B$
					$\hat{T}C = ACB^2$
					$\hat{T}D = A^3B^2D$
					$\hat{P}I = I$
					$\hat{Q}I = I$
					$\hat{R}I = I$
					$\hat{S}I = I$
					$\hat{T}I = I$

6. CONCLUSIONS

In this report, we have reviewed the group-theoretic properties of phase transitions and demonstrated that the problem of extending a group reduces to that of determining its automorphisms.

The automorphism groups of the crystallographic and icosahedral point groups have been derived with a consistent presentation. These new results, which are presented in Tables 6–10, enable the derivation of all extensions of the crystallographic point groups.

Further reports in this series will use this information to identify all spectroscopically-active soft modes for the 230 space groups. Identification of these soft modes will enable a detailed examination of phase transitions in materials of interest to the Canadian Nuclear Program and aid in the optimization of material properties.

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