Clebsch-Gordan Coefficients and Electron-phonon Scattering in the Valence Band of Ge (O_h^7)

Mapingire Hezekia

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Declaration

I sincerely and truthfully declare that this dissertation which I hereby submit for the degree of Master of Science (Physics) at the University of Pretoria is my bona-fide work. The dissertation has not been previously submitted by me or any other individual for any degree at the University of Pretoria or any other institution.

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Abstract

In this work we deduce the types of phonons that take part in scattering electrons from the Brillouin zone (BZ) edge of germanium at the critical point L_3^- to the BZ centre at high symmetry point Γ_{25}^+. Ge semiconductor has the diamond structure and is a member of the O_h^7 space group. The scattering of electrons by phonons in Ge and other similar crystals is a phenomenon that is of critical importance in comprehending the mobility of charge carriers and other significant transport phenomena. Further understanding of the electron-phonon scattering process in Ge and other similar crystals is pertinent because of the possibility of opening new ground in terms of improving the perfomance and efficiency of modern electronic devices made from these semiconductors. Commencing from the Kronecker product $\left(L_3^-\right)^{e^-_{initial}} \otimes \left(\Gamma_{25}^+\right)^{e^-_{final}} = L_1^- + L_2^- + 2L_3^-$, we use group theoretical techniques to compute Clebsch-Gordan coefficients (CGCs) that are utilised to interpret the scattering of electrons from the critical symmetry point L_3^- to the critical symmetry point Γ_{25}^+ within the valence band of Ge. We found out that when electrons are scattered by phonons from the BZ edge of Ge, at point L_3^- to the BZ centre, point Γ_{25}^+, both the longitudinal acoustic (LO) and transverse optical (TO) phonons are present but it is only the TO phonons that participate in this sacttering process. The longitudinal optical (LO) phonons are non-existent in these types of transitions in Ge bands. Our theoretical results are consistent with the experimentally obtained phonon dispersion curves for Ge.

Chapter 1

Introduction

The main objective of this work is to determine the types of phonons that are involved in scattering electrons from the Brillouin zone[1] (BZ) edge of germanium (Ge), at high symmetry point L_3^-, to the BZ centre- high symmetry point Γ_{25}^+. Electron-phonon interaction is a primary source of scattering in nano-devices. The transport properties of Ge based nano-devices and other similar conductors depends on the electron-phonon interactions[1].

We use Clebsch-Gordan coefficients (CGCs) to deduce the types of phonons that take part in this electron-phonon scattering phenomenon. In this work the CGCs that are used to comprehend and interpret this scattering phenomenon are explicitly derived. Electrons can be scattered by phonons from one energy band to another or within the same energy band- that is inter-band and intra-band scattering respectively. An energy band is a spectrum of energy levels that form a continuous range of energy values available for charge carriers. Phonons are ionic motions or quanta of lattice vibrations.

The calculated CGCs in this work are used to interpret the intra-band scattering of electrons by phonons in the valence band of Ge from the critical point L_3^- to the high symmetry point Γ_{25}^+. The CGCs or coupling constants are also utilised to determine the allowed or forbidden phonon transitions within the valence band of Ge.

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[1] The concept of the BZ and symmetry considerations are dealt with in chapter 2.

The use of Clebsch-Gordan coefficients is a powerful group theoretical technique that is widely used to explain theories for a number of phenomena. Among other processes, Clebsch-Gordan coefficients can be used in the derivation of elements of tensors for Brillouin scattering, description and derivation of "morphic induced" Raman scattering[2]. Coupling constants are also utilised in the diagonalisation of phonon dynamical matrices, the description of Gunn effect and the construction of the Hamiltonian matrix elements[3].

This work is also in the form of an incremental improvement in comprehending radiative transitions as well as inter-valley and intra-valley scattering phenomena in Ge[2] using apt selection rules[4]. Selection rules or transition rules govern the transition of charge carriers from an initial quantum mechanical state to another in crystals. The transition rules are of fundamental importance as they are a pre-requisite in the computation of coupling coefficients for crystals[5].

The coupling constants are of utmost importance as they are related to elements of scattering tensors which enable one to comprehend the scattering phenomena in crystals[6]. The scattering processes in crystals have a significant bearing on the mobility of charge carriers and other transport phenomena. A number of investigations on Ge and other similar crystals are focusing on obtaining apt conditions that can be used to obtain maximum carrier mobility in order to increase the perfomance and efficiency of Ge devices. Further understanding of the transport phenomena in Ge and other similar crystals is pertinent as it can lead to an even wider application of these semiconductors especially in the making of opto-electronic devices and modern electronic components.

Ge semiconductor is a member of the O_h^7 space group[3]- diamond structure. The space group of a crystal gives all the possible symmetry properties of the crystal.[4]. The Ge point group is the cubic group O_h. The O_h^7 space group has 48 by 48 symmetry elements.

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[2] Inter-valley and intra-valley scattering phenomena are explored in Chapter 3

[3] O_h^7 is the Schonflies notation. The space group number is 227 and the full international notation is F4_1/d$\bar{3}$2/m.

[4] In three dimensions there are 230 space groups and 32 crystallographic point groups

Applying group theoretical knowledge of the O_h^7 space group to Ge semiconductor, we analyse the first Brillouin zone of this crystal as well as its electronic band structure in chapter 2. This is of fundamental importance as the optical and electrical properties of any crystal hinges on the structure of the BZ and the energy bands of the crystal. The layout of the rest of this dissertation is as follows- we explore the phenomenon of electron-phonon scattering in Ge and the group theoretical techniques applied to this process in chapter 3. In chapter 4 we discuss selection rules for Ge before the derivation of CGCs in chapter 5. We will then present the calculated CGCs that are used to understand the scattering process of electrons by phonons from the BZ edge at point L_3^- to the BZ centre at high symmetry point Γ_{25}^+. The last two chapters of this dissertation are the discussion of results and conclusion respectively. This will then be followed by the appendices section.

Chapter 2

Symmetry and energy band structure of Ge

In this chapter we analyze symmetry transformation before we briefly delve into the fundamental concept of groups. We discuss the concept of the Brillouin zone and the electronic band structure of Ge. In order to understand the properties of a given crystal, we have to comprehend the BZ of the crystal and the electronic energy bands as they have a strong bearing on the the optical and electrical properties of the material.

2.1 Symmetry transformation

We define a symmetry transformation as an operation on a crystal or part of a crystal that leaves the crystal unchanged. The crystal is exactly the same as it was before the operation was carried out [7]. Some fundamental symmetry operations that leaves a crystal in the same positions as before are:

i. C_n- denotes rotation of a crystal about a given axis through a specified angle, $\frac{2\pi}{n}$: If we repeat this application the symmetry transformation will be denoted by C_n^p where p, z are integers. For instance C_3^2, means rotation by $\frac{2\pi}{3}$ and this transformation is done two times;

ii. E- is the identity symmetry transformation: Following the procedure above n

successive rotations about a given axis through the angle $\frac{2\pi}{n}$ yields the identity operation $E = C_n^n$;

iii. i- is the inversion symmetry transformation: For this transformation we have $i(x, y, z) \rightarrow (-x, -y, -z)$ and the crystal appears as it was before even after an inversion through an origin called the centre of inversion;

iv. σ-denotes reflection: we can have a mirror reflection in a given plane, for instance, σ_h and σ_v stands for reflection in the horizontal and vertical plane respectively;

v. t-is translation or parallel displacement of the crystal : for this transformation we assume that the crystal lattice is infinite.

All symmetry transformations of a finite solid crystal must leave at least one point of the crystal fixed or unchanged. The fixed point does not move during the symmetry operation. If many symmetry operations can be done with respect to this point, we refer this point as a critical symmetry point or high symmetry point. Likewise the axis of highest symmetry of a crystal or molecule is called the principal axis. A three-fold axis, for example, implies that there are three symmetry operations about that axis under consideration. Some crystals do not have a principal axis.

Crystals have symmetry because they are formed from a unit cell called the primitive cell in a direct lattice. The primitive cell of the reciprocal lattice- the Brillouin zone (BZ)- is of paramount importance when using symmetry to study crystal properties because it forms the whole lattice structure by symmetry transformations. Within and around the BZ we have fundamental symmetry operations that can be used to comprehend the physical behaviour of crystals in different directions- anisotropy [7]. Symmetry operations form groups when they act on a set of given members. In the next section we briefly explore the concept of groups.

2.2 Group (G)

A group is a set of members that have a common law of operation that can be applied on all the group members such that four fundamental axioms of associativity, closure, identity and inverse hold. Associativity implies that the outcome of a series of operations on given group members is the same even if we change the grouping of the elements as long as we keep the order of the elements constant. For instance, if $g, h, k \in G$ we have $g*(h*k) = (g*h)*k$, where $*$ denotes the group operation such as a symmetry operation. Closure in a group means that the product of any two members of the group must give an outcome of a member that is already in the group, that is $g * h \in G$. In every group there must be an element that does not change anything when it operates on any given group member. This symmetry element is the identity and it is of critical importance in comprehending some group theoretical concepts. Therefore, for each member of a group, $g \in G$, we have $g * E = E * g = g$, where E denotes the identity element. Every element in a given group has an inverse that reverses or undoes the work of each member. For an element g, we have an inverse g^{-1}, which satisfies $g * g^{-1} = g^{-1} * g = E$. A given set of members together with their law of operation is a group if all the four axioms are true. A complete table of composition for all the group members forms a group table or multiplication table which is crucial in understanding the properties of group members. In this work, our crystal of interest- Ge- belongs to the point group O_h and space group O_h^7. The space group of a crystal gives all the possible symmetry properties of the crystal. Fundamental to understanding the properties of a given crystal lies in comprehending the symmetry properties of the Brillouin zone of the given crystal.

2.3 The Brillouin zone

Any space group is made up of an invariant sub-group of primitive translations that are of the form

$$\{\varepsilon \mid R_n\}$$

and

$$R_n = n_1\vec{t_1} + n_2\vec{t_2} + n_3\vec{t_3} \tag{2.1}$$

where n_1 ,n_2 and n_3 are integers and n denotes the collection of the three integers;

$\vec{t_1}$, $\vec{t_2}$ and $\vec{t_3}$ are the basic primitive translation that are linearly independent.

The collection of the entire points that are generated by the vectors R_n is referred to as the crystal lattice. The primitive translations can be given in the form hereby stated

$$\{\varepsilon \mid R_n\} = e^{\left(i\vec{k}.R_n\right)} \tag{2.2}$$

where

$$\vec{k} = k_1\vec{b_1} + k_2\vec{b_2} + k_3\vec{b_3} \tag{2.3}$$

$\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$ are the primitive vectors;

$\vec{k}$ is a vector that forms or generates irreducible representations of the pure translations group.

The crystal space that is spanned by the vectors $\vec{b_1}$, $\vec{b}_2$ and $\vec{b_3}$ is called the reciprocal space. The smallest repeating space or unit cell of the reciprocal space is called the Brillouin zone[8]. In reciprocal space a solid crystal structure is composed of these fundamental identical periodic regions- the Brillouin zones. Apt transformations of the Brillouin zone forms the entire crystal structure. Some of the symmetry transformations that are of critical importance are translation operations, reflections, rotations and a combination of these. The BZ is invariant under these symmetry operations of the space group of the crystal under consideration.

The concepts that are true throughout the entire BZ are also true for the entire crystal structure. The BZ comprises high symmetry points and lines which are critical in comprehending the processes that happen in a semiconductor. Figure 2.1 is an example of the first BZ of the body-centred cubic lattice showing high symmetry points and lines [8]. In this work we have considered the first BZ because it is simple yet has all the relevant physical information required to comprehend scattering processes in a given crystal.

The point Γ is the origin or centre of the Brillouin zone as depicted by figure 2.1.

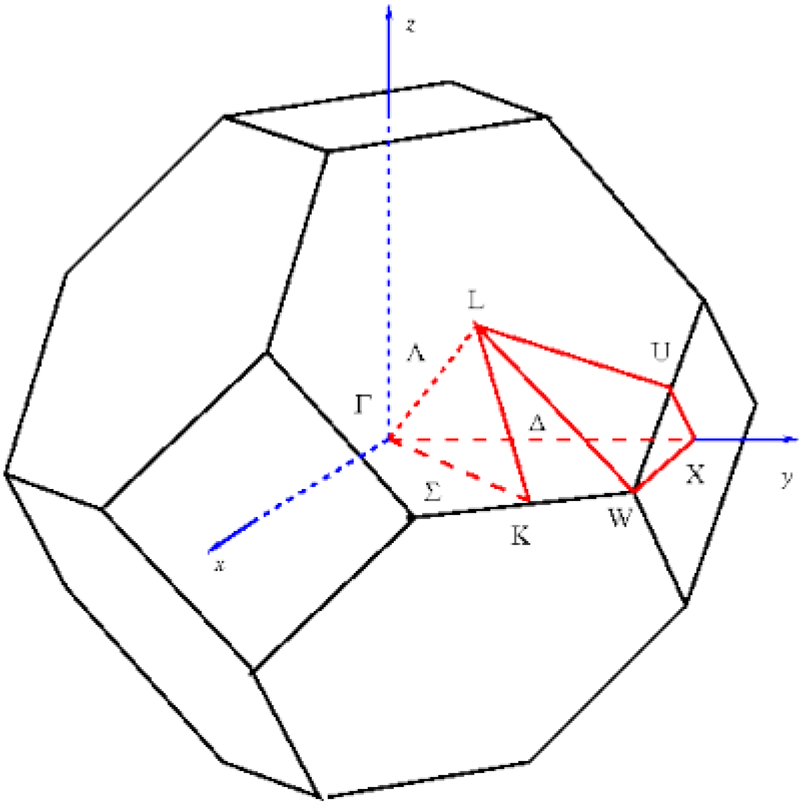

Figure 2.1: The first Brillouin zone of the body-centred cubic lattice crystal structure showing the high symmetry lines and points [8]

The irreducible representations of the entire space group O_h^7 are the irreducible representations of the group of transformations at point Γ, that is G^{k_Γ}[8] . The symbols Δ, Λ and Σ represent or shows the lines within the BZ. The line Σ is a bisector of the angle between the k_x and k_y axes. The points K, W, X, U and L are situated on the surface of the BZ. The high symmetry points and lines have different but equivalent labelling as shown by table C.1 in appendix C[9][10][11]. We use coordinates as depicted by table D.1 in appendix D[11], to indicate the positions of these critical points on the BZ.

After constructing the Brillouin zone, we can have a k-vector that is in or on the surface of the BZ. If the k-vector is allowed to move in the interior and surface of the BZ by symmetry transformation, we get a sub-group of operations of the space group which leaves the k-vector unchanged or send it into one differing by a primitive translation of the reciprocal lattice. The specification of the irreducible representations of the sub-group, for instance G^{k_L}- the sub-group at point L, completely gives the irreducible representations of the entire group G^{k_Γ}[8].

2.4 Energy band structure of Ge

An isolated atom has a number of energy states available for charge carriers. In a crystal, we have many atoms that are close together so that a large number of energy levels exist for charge carriers. We define an energy band as a range of energy states that can be occupied by charge carriers. Two energy bands that are important are the valence and conduction bands because they play a significant role in the mobility of charge carriers in a material. The valence band is the highest occupied energy band in a material at absolute zero temperature. The conduction band is the next band above the valence band which has a range of energy states that charge carriers can occupy. In the conduction band, charge carriers are freely mobile and are capable of producing a current. The valence band is separated from the conduction band by an energy gap or forbidden gap where there are no energy levels available for electrons.

An energy band that is completely filled or empty band cannot have an electric current. The conduction of electric current in a material is due to the motion of electrons and holes in the conduction and valence bands. An insulator is a large band gap material which has no electrons or holes available for the conduction of electric current. An intrinsic semi-conductor behaves like an insulator at absolute zero temperature. We can thus define a semiconductor as a small band gap insulator at absolute zero. At this temperature the conduction band is empty whereas the valence band is completely filled hence there is no possibility of having current flow. If the temperature of a semiconductor is increased, electrons undergo transition from the valence band to the conduction band. This creates a partially filled conduction band that contains thermally excited electrons available for conduction. The transition of electrons from the valence band to the conduction band creates vacant orbitals or holes in the valence band. The holes also contribute to the conduction of electricity. Therefore the total contribution to electrical conductivity is due to the presence of both electrons and holes in the conduction and valence bands respectively. In metals, the valence and conduction bands overlap, hence they are very good conductors of heat and electricity.

Ge is an indirect band gap crystal material as shown by figure 2.2[12]. An indirect band gap semiconductor is one in which the conduction band edge and the valence band edge occur at different locations and directions in reciprocal space. The conduction band edge of Ge is along the $\langle 111 \rangle$ direction. The minimum in the conduction band of Ge is located at the point $L(\frac{\pi}{2})\langle 111 \rangle$ on the BZ boundary. The symmetry of this critical minimum is L_1^+.

The conduction band edge comprises four degenerate pairs of L-valleys along the $\langle 111 \rangle$ direction[13]. The four degenerate valleys have wave vectors whose directions are $\langle 111 \rangle$, $\langle \bar{1}11 \rangle$, $\langle 1\bar{1}1 \rangle$ and $\langle 11\bar{1} \rangle$ as depicted by figure 2.3[14]. The valence band edge is at the zone centre at point $\Gamma\,\langle 000 \rangle$ and has symmetry of Γ_{25}^+.

Ge crystal structure is a lattice that has two atoms in a given unit cell. The atoms are positioned at $(0, 0, 0)$ and $\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$ in the unit cell $(a = 5,6575A)$. This semiconductor belongs to the diamond crystal structure which is composed of two identical face-centred

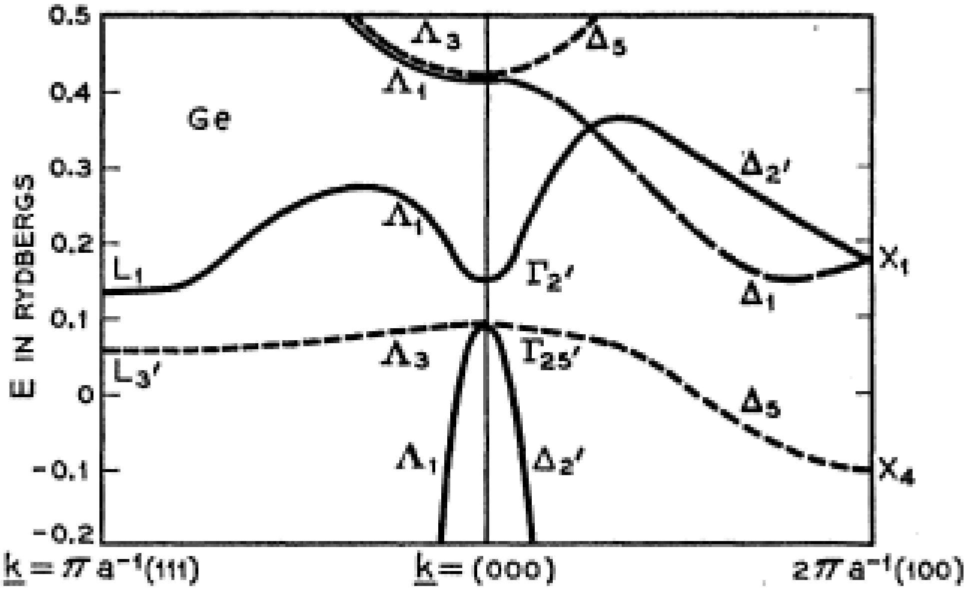

Figure 2.2: The energy band structure of Ge showing the critical symmetry points [12]

cubic lattices which are interpenetrating[14]. At absolute zero temperature, the valence band of Ge is separated from the conduction band by an energy gap of approximately 0.67eV. The energy gap, E_g, which gives us the forbidden states changes with temperature. As illustrated by figure 2.2 , for Ge and other similar crystals, two bands converge at the valence band edge at the BZ centre. These bands are referred to as the heavy- and light-hole bands.

Charge carriers such as electrons can undergo transitions from one high symmetry point to another in the electronic energy bands of Ge as a result of interactions with quasi-particles such as photons and phonons. We discuss electron-phonon scattering phenomena in Ge semiconductor in the next chapter of this dissertation.

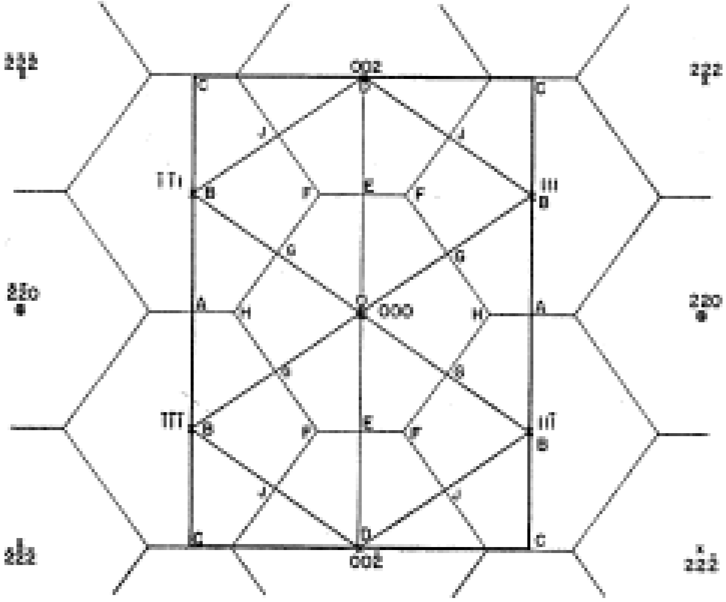

Figure 2.3: The $(1\bar{1}0)$plane of the germanium reciprocal lattice [14]

Chapter 3

Scattering in Ge

A number of investigations on Ge and other similar crystals are focusing on obtaining apt conditions that can give rise to an improvement in carrier mobility in order to increase the perfomance and efficiency of Ge devices. The model of carrier transport developed for Ge in order to comprehend the transport phenomena in this semi-conductor is the intra-valley and inter-valley scattering between its four energy minima. In this chapter we would like to briefly explore intra-valley and inter-valley scattering in Ge and the scattering of electrons and holes by phonons.

3.1 Intra-valley and inter-valley scattering

We define scattering as the transition of charge carriers from an initial quantum mechanical state to another as a result of their interaction with different excitations such as photons, phonons, other carriers, impurities, surfaces, inter-surfaces, defects and also because of the presence of pressure gradient, temperature gradient , electrical field gradient and other field gradients within a solid crystal[13].

Scattering is divided into two classes, which are intra-valley[1] and inter-valley scattering. Intra-valley is the scattering of carriers within the same valley or between valleys that belong to the same star. Star is a collection of valleys that have the same number

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[1] The term valley refers to energy minimum

of carriers and energy and hence are considered to be equivalent. Inter-valley scattering is the transition of carriers from one energy valley to another valley that do not belong to the same star in k-space. Inter-valley scattering is classified into g- and f-scattering processes that are outlined in the next sub-section.

3.1.1 g- and f-scattering

For g-scattering, carriers are scattered from an initial valley to another on the opposite side of the same axis as shown by figure 3.1[15]. The g-process is denoted by q_g and for this phenomenon the two valleys have the same orientation. During the f-scattering process, carriers are scattered the first valley to another one that has a different orientation. The f-scattering phenomenon is denoted by q_f as illustrated by figure 3.1. If the electron valley lies in the same BZ after the scattering process, then such a process is called a normal process. In contrast if the electron valley lies in an adjacent BZ after scattering phenomenon, then the process is called umklapp[13]. Figure 3.2 depicts two adjacent Brillouin zones that can be used to describe a normal or an umklapp process.

Germanium semiconductor is composed of four energy valleys as illustrated by figure 3.3 [16]. The scattering processes in germanium encompass the transition of charge carriers between the four energy valleys. All possible electron-phonon scattering processes and other transport phenomena in Ge depends on what transpires in these constant energy valleys.

3.2 Group theoretical techniques applied to scattering

The states of particles or quasi-particles that are involved in the scattering phenomena are represented by wave functions or state vectors in a Hilbert space. The wave functions contains the possible measurable information of the system under consideration. Some of the physically measurable observables carried by the wave functions includes the displacement, frequency, energy, momentum and the wavevectors of the particles participating in the scattering processes. Utilising symmetry principles, the wave func-

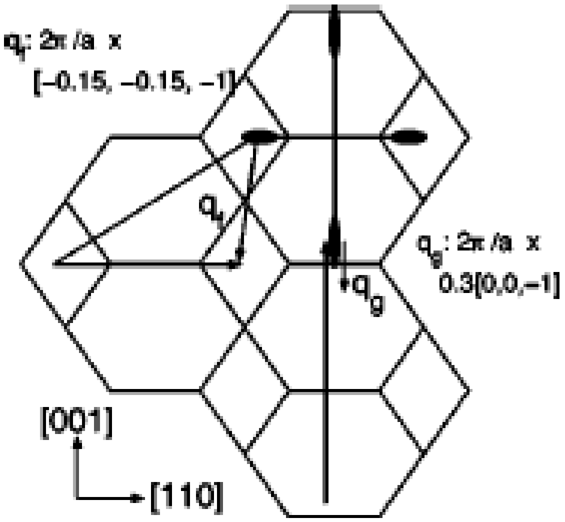

Figure 3.1: Diagram to illustrate g- and f-scattering phenomena in a (110) plane [15].

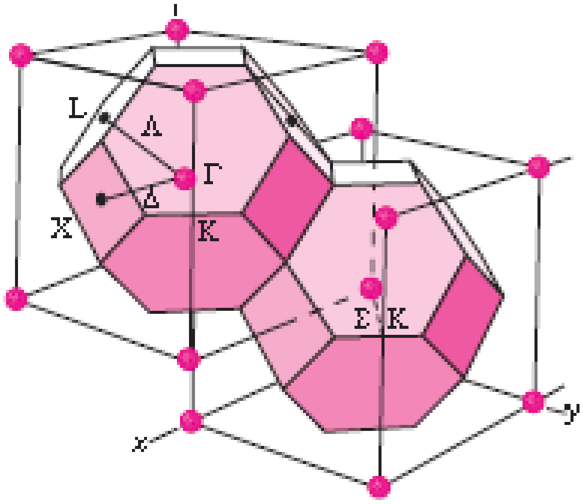

Figure 3.2: Two adjacent Brillouin zones that can be used to illustrate normal and umklapp scattering processes [13].

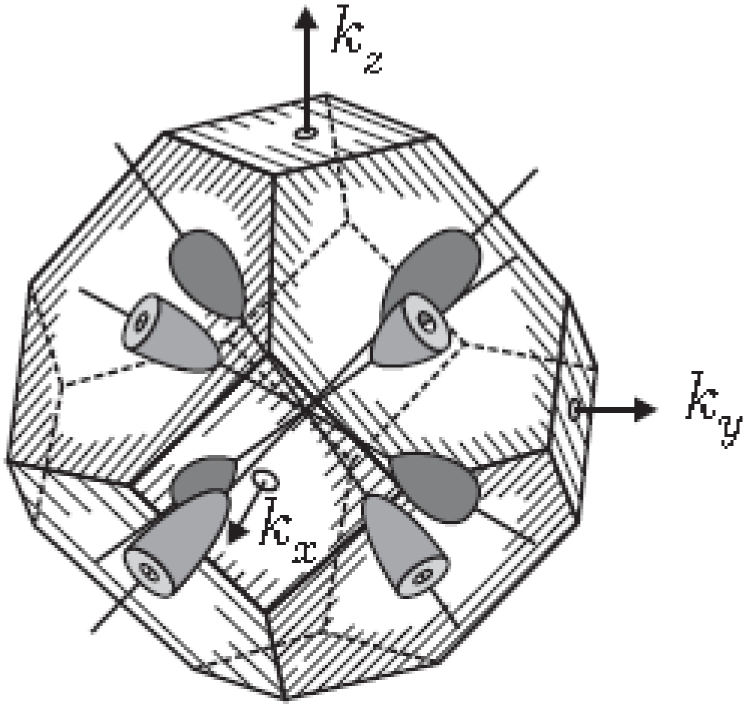

Figure 3.3: The four degenerate L- valleys of Ge [16].

tions are given in a form such that they have transformation properties of the crystal space group under considerations. Such wave functions are said to be symmetrized.

The states of particles and quasi-particles involved in scattering phenomena are represented by irreducible representations of the crystal space group of the semiconductor under considerations. Quasi-particles such as phonons do not have spin. We utilise single-valued irreducible representations (SV irreps) to represent the different states of such quasi-particles. If spin is considered, for example for electrons, the quantum mechanical states of particles of that nature is denoted by mathematical objects called spinors. Spinors are also referred to as double-valued irreducible representations.

During scattering phenomena, the interaction of the particles, for instance electrons and phonons, is represented by Kronecker products (KPs). Inter-valley and intra-valley scattering processes in Ge and other semiconductors are described by using appropriate Kronecker products. The KPs derived from high symmetry points aptly connects the valence band edge and the conduction band edge of the BZ under consideration. Lax and Hopfield[17] pointed out that scattering of electrons from the top of the valence band to the bottom of the conduction band, as depicted in Ge are apt examples of phenomena in which various paramount points of the BZ are intertwined by a perturbation.

For Ge, the high symmetry points on the BZ that among others are of critical importance in describing the scattering processes are $\mathit{\Gamma}, L, \mathit{\Delta}$ and X. The energy, momentum and wavevectors of the particles or quasi-particles are conserved during scattering phenomena. The conservation of these physical quantities that are of critical importance is represented by the wavevector selection rules (WVSRs).

3.3 Scattering of electrons by phonons

The displacement of atoms in the unit cell from their positions of rest will give rise to vibrations or elastic waves that propagate throughout the crystal. These ionic motions or lattice vibrations are called phonons. There are four kinds of phonons, that is transverse acoustic (TA), longitudinal acoustic (LA), transverse optical (TO) and longitudinal optical (LO). The four types of phonons interact differently with electrons and holes during the process of scattering. Scattering of electrons by phonons from the Brillouin zone edge to the zone centre encompass a change in crystal momentum from the initial momentum $\vec{q} \neq 0$ to $\vec{q} = 0$. This crystal momentum must be conserved. In order for this to happen, the electrons can either emit or absorb a phonon that has a crystal momentum of wave vector $\vec{q}$. The phonon spectrum of Ge has four branches in the direction of the conduction band edge. Therefore we have four phonons of different energies that have the apt crystal momentum[18].

3.3.1 Intra-band scattering by phonon emission

We consider an electron of effective mass m^* , initial energy E_i and wave vector $\overrightarrow{k}$. The electron is positioned in a periodic parabolic band and is scattered by a phonon within the same band- intraband scattering. The electron undergoes a transition to another quantum mechanical state of energy E_f and wave vector $\overrightarrow{k'}$. Let us consider a case whereby this phenomenon involves the emission of an acoustic phonon that has energy E_p and wave vector $\overrightarrow{q}$. Since the crystal lattice is periodic , the total energy and wave vectors of the particles or quasi-particles participating in the scattering process are conserved[13]. The energies and wave vectors of the electron and phonon are given by equations (3.1) and (3.2), that is

$final\ energy\ of\ electron - initial\ energy\ of\ electron = energy\ of\ emitted\ phonon$;

$final\ electron\ wave\ vector - initial\ electron\ wave\ vector = wave\ vector\ of\ emitted\ phonon$, i.e

$$E_f - E_i = E_p \tag{3.1}$$

$$\overrightarrow{k'} - \overrightarrow{k} = \overrightarrow{q} \tag{3.2}$$

If the acoustic phonon if of small wave vector $\overrightarrow{q}$, the energy of the phonon is linked to the wave vector by equation (3.3)

$$E_p = \hbar v_s \overrightarrow{q} \tag{3.3}$$

where v_s is the phonon velocity which is considered to be isotropic[13]. The permitted or possible values of the phonon wave vector are obtained by combining equations (3.1), (3.2) and (3.3) to get equation (3.4)

$$\left(\frac{\hbar^2}{2m^*}\right)\left(k^2 - \mid \vec{k} - \vec{q} \mid^2\right) = \hbar v_s \overrightarrow{q} \tag{3.4}$$

If we compute the values that q can take, we deduce that the permissable values of q are entwined between a minimum, q_{min}, and a maximum, q_{max}.[2] In the next sub-section we now consider intra-band scattering by phonon absorption.

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[2] The scattering of electrons by emission of an acoustic phonon is considered to be elastic.

3.3.2 Intra-band scattering by phonon absoption

We consider a normal scattering phenomenon where an electron undergoes a transition from an initial state $\vec{k}$ to a final quantum mechanical state $\vec{k'}$ as a result of the absorption of a phonon that has wave vector $\vec{q}$[19]. If we assume that crystal momentum remains constant and the initial and final electron states are found within the same spherical parabolic band, the phonon absorption depends on equation (3.5)

$$k'^2 = k^2 + q^2 + 2kqcos\theta \tag{3.5}$$

where θ is the angle between initial the wave vector $\vec{k}$ and the final wave vector $\vec{k'}$

$$\frac{\hbar^2 k'^2}{2m^*} = \frac{\hbar^2 k^2}{2m^*} + \hbar\omega \tag{3.6}$$

thus we have

$$cos\theta = -\frac{q}{2k} + \frac{m^*\omega}{\hbar kq} \tag{3.7}$$

Now if we let

$$f\left(q\right) = -\frac{q}{2k} + \frac{m^*\omega}{\hbar kq} \tag{3.8}$$

we have the function

$$f\left(q\right) = cos\theta \tag{3.9}$$

The principles of conservation of energy and momentum imposes the restriction -1$\leqslant$ $f\left(q\right)$ $\leqslant$1 on equation (3.9). For absorption of acoustic phonons, for instance, we have $\omega = \nu_s q$ and $\hbar k = m^*\nu$ thus we get equation (3.10)

$$f\left(q\right) = \frac{-q}{2k} + \frac{\nu_s}{\nu} \tag{3.10}$$

For a particular case where $\nu \geqslant \nu_s$, the minimum value taken by q is 0 and the maximum value of q is given by $f\left(q\right) = -1$[19]. Therefore for phonon absorption, the allowed values of q also lie between a minimum and a maximum.

3.3.3 Born-Oppenheimer electron-phonon interaction

We use the Born-Oppenheimer[3] approximation to describe the scattering phenomena that happens when charge carriers undergo a transition from an initial quantum mechanical state to another as a result of their interactions with phonons or lattice vibrations. For the Born-Oppenheimer approximation to hold, we assume that electrons can respond instantaneously to the lattice vibrations. The ions are regarded as being stationary when compared to the electronic motion. In contrast the ions cannot follow the motion of the electrons. They are considered to be influenced by a time-averaged adiabatic electronic potential. In this approximation, we assume that the electrons follow the ionic motion adiabatically[13].

Utilising this approximation we decompose the Hamiltonian of a crystal into three fundamental terms, that is

$$H = H_{ions}(\vec{R}_j) + H_e(\vec{r}_i, \vec{R}_{jo}) + H_{e-ion}(\vec{r}_i, \delta\vec{R}_j) \tag{3.11}$$

where $H_{ions}(\vec{R}_j)$ describes the atomic displacements under the effect of ionic potentials as well as the time–averaged adiabatic electronic potentials;

$H_e(\vec{r}_i, \vec{R}_{jo})$ is a term that describes the electrons when the ions are assumed to be fixed in their equilibrium positions $\vec{R}_{jo}$;

$H_{e-ion}(\vec{r}_i, \delta\vec{R}_j)$ represents the electron-phonon interaction which brings about a change in the electronic energy because of the displacement of the ions from their positions of rest.

Electron-phonon interactions which give rise to inter-valley and intra-valley scattering can induce changes in the electronic band energy. Phonons or atomic displacements can shift the electronic energies at various points in the Brillouin zone. Charge carriers, for example electrons can interact with zone-center phonons and zone-edge phonons and are continuously scattered within an energy valley or from one energy valley to another-

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[3] The Born -Oppenheimer approximation for electron-phonon interaction is sometimes known as the adiabatic approximation[13].

inter-valley scattering. Understanding of the inter-valley scattering phenomenon requires the computation of the inter-valley electron-phonon Hamiltonian as described in the next section.

3.3.4 Inter-valley electron-phonon Hamiltonian

For inter-valley electron-phonon interactions, the inter-valley electron-phonon Hamiltonian is given by

$$H_{i\nu} = \vec{e}_{b\vec{q}} \cdot \frac{\delta H_e}{\delta R} u \tag{3.12}$$

where $\vec{e}$ is the phonon polarization vector;

u is the amplitude;

$\vec{q}$ is the wave vector of the phonon;

b is the branch number.

Since scattering gives rise to the transition of a carrier from one quantum mechanical state to another, the inter-valley electron-phonon Hamiltonian can be given in terms of its matrix elements between the initial and final electronic states as depicted by equation (3.13)

$$D_{ij} H = \left\langle n_i, \vec{k}_i \left| H_{iv} \right| n_j, \vec{k}_j \right\rangle \tag{3.13}$$

where D_{ij} is the inter-valley deformation potential;

i and j denote respectively the initial and final valleys in the scattering;

n is the electronic band index;

$\vec{k}$ is the wave vector.

The transition of charge carriers from an initial quantum state to another is subject to certain constraints that can either allow or forbid such processes. These constraints that permit certain transitions whilst rejecting or filtering out other quantum mechanical transitions are referred to as selection rules. The selection rules for inter- and intra-valley scattering phenomena in Ge are dealt with in the chapter that follows.

Chapter 4

Selection rules

In this chapter we explore group theoretical selection rules and wave-vector selection rules. We will utilize the selection rules to determine if radiative transition of electrons from the conduction band to the valence band of Ge is allowed. We also use a similar technique to determine the possible intra-band phonon transitions in the valence and conduction bands of Ge.

4.1 Selection rules

The transition of a charge carrier from an initial quantum mechanical state to a new state is controlled by selection rules. Selection rules determine whether a transition is possible or not. There are many mathematically possible transitions of charge carriers from one quantum mechanical state to another. The selection rules filter the transitions that are physically permissable. Understanding of scattering processes in crystalline solids requires the use or computation appropriate selection rules.

Lax and Hopfield[17] pointed out that selection rules are derived from an integral of the form

$$\int \Psi_\lambda^i(k,r)\Psi_\mu^j(k',r)\Psi_v^m(k'',r)^* dr \tag{4.1}$$

where $\Psi_\lambda^i(k,r)$ is a term that represents an initial charge carrier state which has symmetry transformations of the λ^{th} row of the irreducible representation i with wave-vector k;

$\Psi^j_\mu(k', r)$ represents the pertubation state of excitations such as photons, phonons and others- these have symmetry transformations of the μ^{th} row of the irreducible representation j with wave-vector k';

$\Psi^m_v(k'', r)$ represents the final charge carrier state which depicts symmetry transformations of the ν^{th} row of the irreducible representation m with wave-vector k''.

If a transition from an initial quantum mechanical state to another is permitted, the integral gives a non-zero value as the outcome. In contrast if the transition is not allowed, the integral vanishes or gives a zero. The method that is generally utilised to obtain selection rules from equation (4.1) is to use the initial carrier state, the final carrier state or the perturbation representation as a starting point for the construction of a product representation. The product representation is then reduced into a sum of irreps that are contained in the product as depicted by equation (4.2)

$$D^i_\lambda \otimes D^j_\mu = \sum C^{ij,m}_{\lambda\mu,v} D^m_v \tag{4.2}$$

Where $C^{ij,m}_{\lambda\mu,v}$ is a term that denotes the frequency of occurrence of the representation D^m_v in the product $D^i_\lambda \otimes D^j_\mu$.

Therefore the decomposition of products of the irreducible representations of crystal group under consideration yields the frequency of occurrence of each irreducible representation in the product[5, 20]. The selection rules are derived from the eigen-functions of a perturbation, Ψ^j_μ , linking the initial and the final quantum mechanical states of a system under consideration. The eigen-functions or wave functions are of the form

$$V^{ij,m}_{\lambda\mu,\nu} = \left\langle \Psi^i_\lambda \left| \Psi^j_\mu \right| \Psi^m_v \right\rangle \tag{4.3}$$

where Ψ^i_λ and Ψ^m_ν are the eigen-functions or wave functions representing the initial and the final quantum states of the particles or quasi-particles participating in the transition processes.

The corresponding irreps are D^i_λ,D^j_μ and D^m_ν. Using symmetry operators of the O^7_h space group on the wave functions and the perturbation function, Ψ^j_μ, we get the Kronecker product between any two of the three irreps D^i_λ, D^j_μ and D^m_ν. The KP[1] represents the interaction between the particles or the quasi-particles involved in the transition process. The transition between two states is allowed if the product representation is decomposed into direct sum of irreps that contains the identity representation or the third representation not in the product. Consider the KP

$$D^i_\lambda \otimes D^j_\mu = D^m_\nu + D^n_\tau \tag{4.4}$$

The transition is allowed if the product of D^i_λ or D^j_μ with the outcome, $D^m_\upsilon + D^n_\tau$, yields a result that contains the identity representation.

4.2 The wave vector selection rules for Ge

The wave vector selection rules (WVSRs) represent the fundamental principles of energy and momentum conservation in a crystal lattice. Consider for example, a charge carrier in an initial quantum mechanical state k. The charge undergoes a transition to a new state $k^{'}$ due to interaction with say a phonon in a state k''. Crystal momentum is conserved and the momentum conservation principle is expressed in the form depicted by equation (4.5)

$$k'' = k + k^{'} \tag{4.5}$$

As given by Kunert et al [4] the WVSRs for the intra-valley scattering processes in Ge for the four equivalent L-valleys in accordance with the form above, are

$$1k_L + 1k_L = k_\Gamma \tag{4.6}$$

---

[1] The possible KP for the 230 space groups have been tabulated by Cracknell, Davis, Miller and Love[10].

$$2k_L + 2k_L = k_\Gamma \tag{4.7}$$

$$3k_L + 3k_L = k_\Gamma \tag{4.8}$$

$$4k_L + 4k_L = k_\Gamma \tag{4.9}$$

The four equivalent minima at the critical point L are obtained from the star of the wave vector $k_L = \frac{\pi}{a}(1,1,1)$ of the sub-group at this high symmetry point. We use G^{k_L} to represent the sub-group at the L point[4]. The collection of equivalent valleys at this critical symmetry point in Ge is denoted by $*k_L$ where

$$*k_L = Ek_L, C_{2x}k_L, C_{2y}k_L, C_{2z}k_L \tag{4.10}$$

$$C_{2x}k_L = \frac{\pi}{a}(-1,0,0)$$

$$C_{2y}k_L = \frac{\pi}{a}(0,-1,0)$$

$$C_{2z}k_L = \frac{\pi}{a}(0,0,-1)$$

The symmetry operators of the O_h^7 space group transforms the wave vector $k_L = \frac{\pi}{a}(1,1,1)$ into the other equivalent valleys. Using CDML notation, some of these symmetry operators are $E(1)$,$C_{2x}(2), C_{2y}(3), C_{2z}(4)$ and $C_{31}^-(5)$, $C_{31}^+(9)$[10]. For the inter-valley scattering processes that encompass the L and X valleys in Ge, the WVSRs involve the four L-valleys and the three X-valleys[4]. The WVSRs are represented by equations (4.11) , (4.12) , (4.13) , 4.14 , (4.15) and (4.16).

$$1k_L + 3k_L = k_X \tag{4.11}$$

$$2k_L + 4k_L = k_X \tag{4.12}$$

$$1k_L + 2k_L = 5k_X \tag{4.13}$$

$$4k_L + 3k_L = 5k_X \tag{4.14}$$

$$1k_L + 4k_L = 9k_X \tag{4.15}$$

$$2k_L + 3k_L = 9k_X \tag{4.16}$$

The symmetric KPs that have to come into play in order to interpret the scattering phenomena between different valleys belonging to the same star in Ge, are: $[\Gamma_{2'}]_{(2)}$; $[L_{1'}]_{(2)}$; $[\Delta_1]_{(2)}$[17]. Alternatively, this is given by $[\Gamma_{2-}]_{(2)}$; $[L_{1+}]_{(2)}$; $[\Delta_1]_{(2)}$[10]

4.3 Selection rules for optical and intra-band phonon transitions in Ge

There is no direct link between the conduction band edge and the valence band edge of Ge hence a direct transition that conserves the k-vector does not connect the valence band maximum point to the bottom edge of the conduction band. The likely channels of transitions of electron carriers from the conduction band to the valence band are of two forms[17]- case 1 and case 2 as depicted by figure 4.1 and figure 4.2 respectively.

Case I:

An electron could be scattered by a phonon first from L_1^+ to Γ_2^- (intra-band scattering of an electron through phonon participation in the conduction band of Ge) and then undergo another transition radiatively from Γ_2^- (CB) to Γ_{25}^+ (VB).

When an electron gets scattered by a phonon from the high symmetry point L_1^+ to the high symmetry point Γ_2^- within the conduction band of Ge as depicted by figure 4.1, this interaction is aptly represented by the Kronecker product hereby stated[17]

$$L_1^+ \otimes \mathit{\Gamma}_2^- = L_2^- \tag{4.17}$$

When an electron drops radiatively from Γ_2^- (CB) to Γ_{25}^+ (VB) after being scattered by a phonon from L_1^+ to Γ_2^- the Kronecker product for this radiative transition is

$$\Gamma_{25}^+ \otimes \Gamma_{15}^- = \Gamma_2^- + \Gamma_{12}^- + \Gamma_{25}^- + \Gamma_{15}^- \tag{4.18}$$

The KP $\Gamma_{25}^+ \otimes$ Γ_{15}^- contains Γ_2^-, therefore group theoretically we can conclude that the radiative drop is allowed[17].

Case 2:

An electron could undergo a vertical transition or drop radiatively from the conduction band at high symmetry point L_1^+ to the corresponding high symmetry point L_3^- in the valence band. The electron can then be scattered by a phonon from the Brillouin zone edge at point L_3^- to the BZ centre at high symmetry point Γ_{25}^+ - intra-band scattering of an electron through phonon participation in the valence band of Ge.

When an electron drops radiatively from L_1^+ (CB) to L_3^- (VB) at the Brillouin zone edge, as shown by figure 4.2, the eigen-functions that govern the selection rule are of the form

$$\left\langle \Psi_i^{CB} \middle| \hat{O}_{light}^{p} \middle| \Psi_f^{VB} \right\rangle \tag{4.19}$$

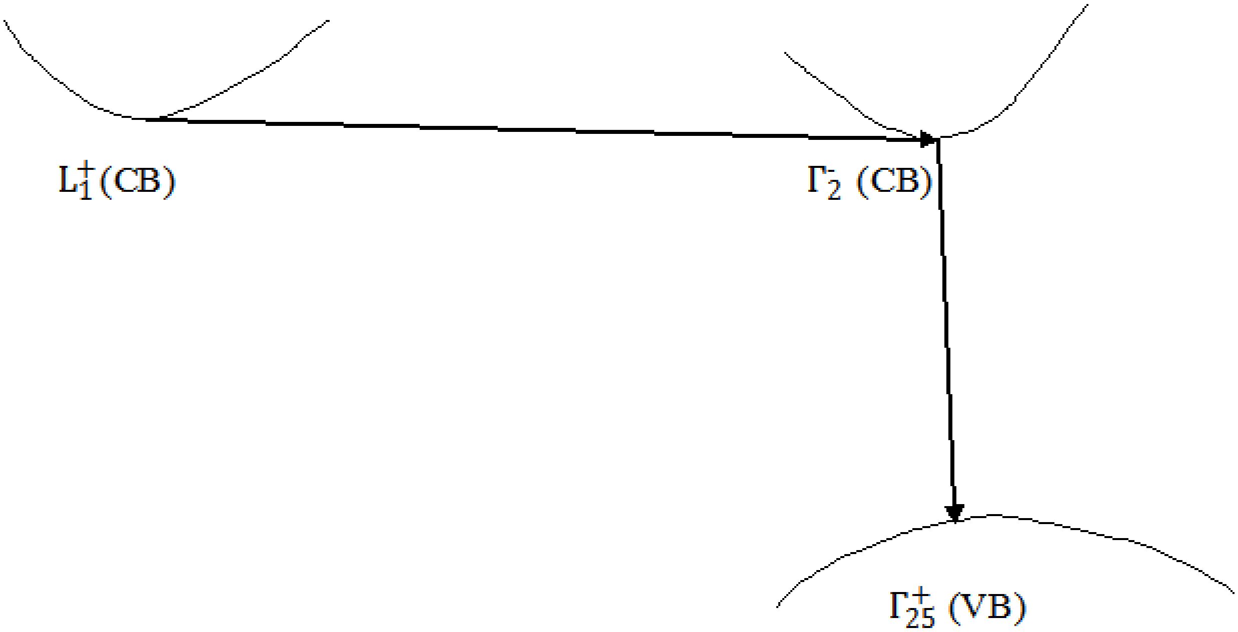

Figure 4.1: CASE 1:The intra-band scattering of an electron by a phonon within the conduction band of Ge from the high symmetry point L_1^+ to Γ_2^- followed by a radiative drop from the conduction band to the valence band- high symmetry point Γ_{25}^+.

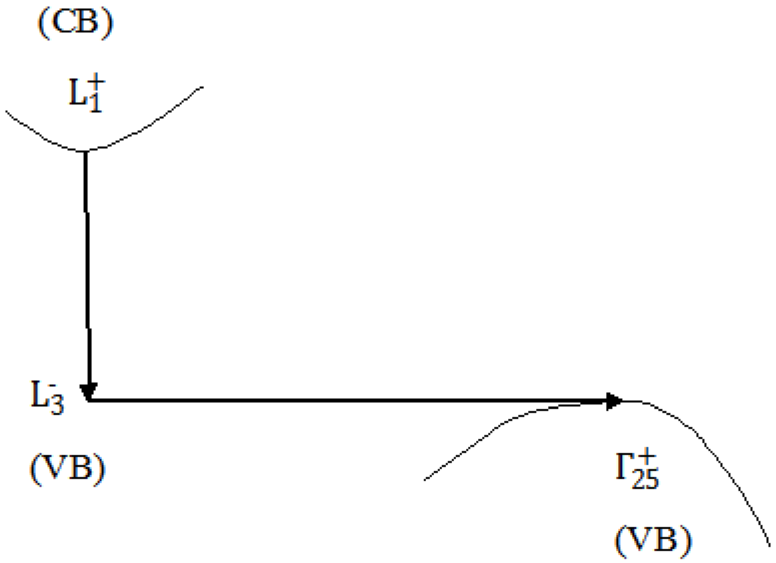

Figure 4.2: CASE 2: Vertical radiative transition of an electron from L_1^+ (CB) to L_3^- (VB) followed by the intra-band scattering of the electron through phonon participation in the VB of Ge

The corresponding selection rule is

$$L_3^- \otimes \Gamma_{15}^- = L_1^+ + L_2^+ + 2L_3^+ \tag{4.20}$$

The product representation $L_3^- \otimes L_{15}^-$ contains L_1^+ which is the identity representation, therefore group theory permits the radiative part of the transition. The symmetry representation Γ_{15}^- denotes the symmetry of light which undergoes transformation like an ordinary vector (x, y, z). This vertical transition is only accompanied by a change in energy since the k-vector is preserved- it remains constant.

For the intra-band electron transition via phonons in the valence band of Ge, an electron is scattered by a phonon from high symmetry point L_3^- at the BZ edge to the BZ centre- point Γ_{25}^+. This transition involves a change in the k-vector and energetic phonons take part since there is a change in the direction of the charge carriers under consideration.

This electron-phonon interaction is denoted by the quantum representation below:

$$\left\langle \Psi_{L_3^-}^{e^-} \middle| \hat{O}_{phonon} \middle| \Psi_{\mathit{\Gamma}_{25}^+}^{e^-} \right\rangle \tag{4.21}$$

Group theoretically the interaction is represented by the Kronecker product hereby stated:

$$(L_3^-)^{e^-_{initial}} \otimes (\Gamma_{25}^+)^{e^-_{final}} = L_1^- + L_2^- + 2L_3^- \tag{4.22}$$

The representations L_1^- , L_2^- and L_3^- on the right side of the KP denotes the phonon symmetry representations anticipated to take part in the valence intra-band phonon transition of electrons in Ge. The phonons represented by the high symmetry points L_1^-, L_2^- and L_3^- are allowed to take part in this transition if quantum mechanical selection rules derived from the initial electron state, final electron state and the perturbation representation (phonon representation), yields an identity representation or the third representation not initially in the product.

The quantum mechanical selection rules that have to be investigated are:

$$\left\langle \Psi_{L_3^-}^{electron} \middle| \hat{O}_{L_1^-}^{phonon} \middle| \Psi_{\mathit{\Gamma}_{25}^+}^{electron} \right\rangle \tag{4.23}$$

$$\left\langle \Psi_{L_3^-}^{electron} \middle| \hat{O}_{L_2^-}^{phonon} \middle| \Psi_{\mathit{\Gamma}_{25}^+}^{electron} \right\rangle \tag{4.24}$$

$$\left\langle \Psi_{L_3^-}^{electron} \middle| \hat{O}_{L_3^-}^{phonon} \middle| \Psi_{\mathit{\Gamma}_{25}^+}^{electron} \right\rangle \tag{4.25}$$

This is investigated by way of the Clebsch-Gordan coefficients or coupling constants which will be derived in the subsequent chapter.

Chapter 5

Computation of Clebsch-Gordan Coefficients

In this chapter we explore the fundamental concepts of Clebsch-Gordan coefficients and the unitary matrix. We commence from the description of the coupling constants before we analyse their utilization in comprehending scattering processes in crystals. This is then followed by a section on the construction of group representations before we delve into a step by step computation of the coupling constants. The derived coupling constants are used to interpret the intra-band scattering of electrons by phonons from the Brillouin zone edge at high symmetry point L_3^- to the zone centre at the critical point Γ_{25}^+ within the valence band of Ge.

5.1 Description of Clebsch-Gordan coefficients

The coupling constants are of utmost importance as they are entwined to elements of scattering tensors which enable one to comprehend the scattering phenomena in crystals[6]. The scattering processes in crystals have a significant bearing on the mobility of carriers and other transport phenomena. Clebsch-Gordan Coefficients are sets of numbers that are used to transform the outer product or tensor product or Kronecker product of two irreducible representations of a group G into a form that is suitable for process interpretation. [1]. The outer product representation is carried by a tensor product space and this can be reduced under the group G. The reduction of the outer product of representations into irreps of G requires a basis transformation of the tensor product spaces.[2]

The basis transformation is accomplished by way of using the unitary matrix. The unitary matrix U is made up of orthonormal bases of Hilbert spaces or tensor product spaces. The transformation from one orthonormal basis to another is done using the unitary matrix[21]. A possible change of basis vectors is thus done by the unitary matrix which preserves orthonormality and this simplifies calculations.

CGCs can therefore be defined as elements of the unitary matrix-U, that decomposes the Kronecker product of two irreducible representations into a sum of blocks of irrps contained in the Kronecker product $D^{\{^*k\}l} \otimes D^{\{^*k'\}l'}$. The unitary matrix transforms the irreps into a completely reduced form by way of the operation given by equation (5.1)

$$U^{-1}D^{\{^*k\}l} \otimes D^{\{^*k'\}l'}U = \sum_{l''} C_{ll'}l''D^{\{^*k''\}l''} \tag{5.1}$$

Where D is the representation of a given wavevector,

U is the unitary matrix that transforms the KP of two irreps into a fully decomposed form;

$^*k,^*k',^*k''$ are the stars[3] of the wavevectors k , k' and k'' respectively.

The unitary matrix or CGCs matrix gives basis functions of irrps (l'') permitted by symmetry in terms of product wave functions $l \otimes l^{'}$. The unitary matrix also diagonalizes any KP of two irrps $l \otimes l^{'}$ and transfoms the irrps l'' to the diagonal block form matrix[21]. CGCs can also be explained as coefficients entwined between basis functions of the irreps contained in the KP and the basis functions of the product of the of the two irreps.

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[1] We define a group as a set of symmetry elements that has a law of combination which is applicable to all the group elements in such a way that four fundamental axioms- associativity, identity, inverse and closure hold.

[2] Reduction of a representation is the process of producing a number of representations that are smaller in terms of dimensions from those that have higher dimensions

[3] A star is a collection of valleys that have an equal number of charge carriers and have the same energy hence they are equivalent.

The irreps denotes the states of the particles that take part in a scattering process[6] . Mathematically, the above concepts are given by the equation (5.2)

$$\Psi^{k''_{\sigma''} l''\gamma}_{a''} = \sum_{\sigma a}\sum_{\sigma' a'} \begin{pmatrix} klk'l'|k''l''\gamma \\ \sigma a\sigma' a'|\sigma'' a'' \end{pmatrix} \phi^{k_\sigma l}_{a} \phi^{k'_\sigma l'}_{a'} \tag{5.2}$$

The matrix elements of the Clebsch-Gordan coefficients are given by equation (5.3)

$$\begin{pmatrix} klk'l'|k''l''\gamma \\ \sigma a\sigma' a'|\sigma'' a'' \end{pmatrix} = U^{\sigma l\sigma' l';\sigma'' l''\gamma}_{aa';a\prime\prime} \tag{5.3}$$

Where $a, a^{'}$ are the matrix elements of the KP $l \otimes l^{'}$,

a'' are the matrix elements of the representation l'', contained in the product $l \otimes l^{'}$

$k, k^{'}$ and k'' are the wavevectors of the particles participating in the scattering processes.

5.2 Clebsch-Gordan coefficients in scattering

Birman and Berenson[6] showed the use of CGCs to comprehend scattering processes.They described the phenomenon of light scattering brought about by quasi-particles such as phonons in a crystal lattice. They utilised coupling constants to interpret this phenomenon. They considered photons incident on a solid crystal and polarised in the direction β . If the scattered photons are polarised in a different direction ,α, then the intensity of the scattered light is given by equation (5.4)

$$I = C \mid \epsilon_{2\alpha} P_{\alpha\beta} \epsilon_{1\beta} \mid^2 \tag{5.4}$$

where C is a constant,

$\epsilon_{2\alpha}$ refers to the Cartesian components of the scattered light whereby α= 1,2,3,

$\epsilon_{1\beta}$ refers to the Cartesian components of the incident radiation whereby β= 1,2,3,

$P_{\alpha\beta}$ is a scattering tensor and it relates the incident radiation to the outgoing scattered radiation.

In line with equation (5.4), the intensity for a first order one excitation process is given by equation (5.5)

$$I' = C' \mid \epsilon_{2\alpha} P^{(1)}_{\alpha\beta} \, (j\sigma) \, \epsilon_{1\beta} \mid^2 \tag{5.5}$$

where $j\sigma$ denotes the symmetry of the excitation under consideration.

The excitations under consideration can be phonons, magnons, polaritons and so on. For scattering of light by phonons, $j\sigma$ represents the symmetry of the phonons for the first order phenomenon. Likewise, if we consider a second order or two excitation phenomenon, the intensity will be given by equation (5.6)

$$I'' = C'' \mid \epsilon_{2\alpha} P^{(2)}_{\alpha\beta} \left(j\sigma; j'\sigma' \right) \epsilon_{1\beta} \mid^2 \tag{5.6}$$

The terms $j\sigma; j'\sigma'$ shows that we are dealing with a second order or two excitation process and they represent the symmetry of the excitations under consideration. In order to comprehend the scattering phenomena, Birman and Berenson[6] put into consideration the symmetry of the crystal and the transformations of various elements in the lattice structure. These two important aspects of the scattering phenomena are dealt with in the sub-section that follows.

5.2.1 Crystal symmetry considerations

The symmetry of the space group to which the crystal lattice belongs is of critical importance in describing the scattering process. The transformation of any symmetry element in the given space group, G, is described by equation (5.7)

$$S = \left(\Phi_s \mid \vec{t_s} \right) \tag{5.7}$$

where S denotes a symmetry element in the crystal space group G;

Φ_s is a rotation transformation which is orthogonal;

$\vec{t_s}$ represents a translation symmetry in the lattice.

If the rotation, Φ_s, is considered to be an orthogal matrix where $S^{-1}_{\lambda\mu} = S_{\lambda\mu}$, we have the following transformations

$$\vec{r} \xrightarrow{s} \vec{r'_s} = \Phi_s \vec{r_s} \tag{5.8}$$

$$r_\mu \xrightarrow{s} r'_\mu = \sum_\lambda S_{\mu\lambda} r_\lambda \tag{5.9}$$

$$\hat{\epsilon_j} \xrightarrow{s} \hat{\epsilon'_j} \tag{5.10}$$

$$Q^j_\sigma \xrightarrow{s} Q^{j'}_\sigma = \sum_\tau D^{(j)}\left(S\right)_{\tau\sigma} Q^j_\tau \tag{5.11}$$

$$P_{\alpha\beta}\left(\vec{R}\right) \xrightarrow{s} P'_{\alpha\beta}\left(\vec{R}\right) = \sum_{\lambda\mu} S_{\alpha\lambda} S_{\beta\mu} P_{\lambda\mu}\left(S^{-1}\vec{R}\right) \tag{5.12}$$

where $\vec{r}$ is a polar vector which transforms like the polarization vector $\hat{\epsilon_j}$;

$\hat{\epsilon}$ is a unit polarization vector;

Q^j_σ denotes the normal coordinates of the crystal lattice;

$\vec{R}$ denotes the displacement of ions from their equilibrium positions as a result of the scattering process and is given by $\vec{R} = \vec{R^0} + \vec{u}$;

$\vec{u}$ is a displacement vector.

5.2.2 Link between Clebsch-Gordan coefficients and scattering tensors

The scattering tensor term, $P_{\alpha\beta}$, can be given in the form of Taylor expansion as shown by equation (5.13),

$$P_{\alpha\beta}\left(\vec{R}\right) = P^{(0)}_{\alpha\beta}\left(\vec{R^0}\right) + \sum_{j\sigma} P^{(1)}_{\alpha\beta}\left(\vec{R^0};j\sigma\right) Q^j_\sigma + \sum_{jj'}\sum_{\sigma\sigma'} P^{(2)}_{\alpha\beta}\left(\vec{R^0};j\sigma;j'\sigma'\right) Q^j_\sigma Q^{j'}_{\sigma'} + \ldots \tag{5.13}$$

The terms linear in Q^j_σ yields a one phonon scattering process while the bilinear terms

$Q^{j}_{\sigma}Q^{j'}_{\sigma'}$ gives a two phonon scattering process. $P_{\alpha\beta} = P_{\beta\alpha}$ since the scattering tensor used to describe phonons is symmetric and because of crystal symmetry $P_{\alpha\beta} = P'_{\alpha\beta}$. The operators in equation (5.13) transform as a second-rank Cartesian tensors and are given by equations (5.14) and equations (5.15) and (5.16) in the first and second order respectively.

$$P_{\alpha\beta}\left(\vec{R}\right) = \sum_{\lambda\mu} S_{\alpha\lambda}S_{\beta\mu}P_{\lambda\mu}\left(S^{-1}\vec{R}\right) \tag{5.14}$$

$$P^{(1)}_{\alpha\beta}\left(j\sigma\right) = \sum_{\lambda\mu} S_{\alpha\lambda}S_{\beta\mu}\sum_{\tau} D^{(j)}\left(S^{-1}\right)_{\tau\sigma} P^{(1)}_{\lambda\mu}\left(j\tau\right) = \sum_{\lambda\mu}\sum_{\tau} S_{\alpha\mu}S_{\beta\mu}D^{(j)}\left(S\right)^{*}_{\sigma\tau}\left(j\tau\right) \tag{5.15}$$

$$P^{(2)}_{\alpha\beta}\left(j\sigma;j'\sigma'\right) = \sum_{\lambda\mu}\sum_{\tau\tau'} S_{\alpha\lambda}S_{\beta\mu}D^{(j)}\left(S\right)^{*}_{\sigma\tau}\left(j\tau\right)D^{(j)}\left(S\right)^{*}_{\sigma'\tau'} \times P^{(2)}_{\lambda\mu}\left(j\tau;j'\tau'\right) \tag{5.16}$$

Birman and Berenson[6] utilised these equations as a basis for the derivation of scattering tensor elements. After manipulating these equations, they came up with a crucial link between Clebsch-Gordan coefficients and elements of scattering tensors. For instance, for the first order phenomenon the relationship is given by equation (5.17).

$$P^{(1)}_{\alpha\beta}\left(j\sigma\right) = \sum_{\lambda\mu\tau} U_{\alpha\beta j\sigma}U^{-1}_{j\tau\lambda\mu}P^{(1)}_{\lambda\mu}\left(j\tau\right)\frac{1}{l_j} \tag{5.17}$$

where l_j represents the dimension of the irreducible representation $D^{(j)}$;

U is the Clebsch-Gordan coefficients matrix.

Therefore, the elements of the first order scattering tensor are actually Clebsch-Gordan coefficients multiplied by a consant. Moreover Birman and Berenson[6] further proved that elements of the second-order scattering tensor are bilinear sums of Clebsch-Gordan coefficients. In order to comprehend sacttering processes, the computation of the Clebsch-Gordan coefficients is therefore of paramount importance as they are utilised in interpreting scattering processes. We hereby compute the coupling constants in the section that follows.

5.3 Derivation of Clebsch-Gordan coefficients

In order to derive Clebsch-Gordan coefficients the initial stage is the construction of group representations for the space group under consideration. In this case we need the irreducible representations for O_h^7 space group. The derivation of the matrix representations for the particles or quasi-particles participating in the scattering process requires the following:

- Symmetry elements of the group under consideration – the symmetry elements and the group are analogous to vectors in a linear vector space;
- Generators or augumenters for the derivation of all the group members - the generators are analogous to the basis vectors that span a vector space;
- The BZ of the O_h^7 space group that shows the critical symmetry points and lines;
- The electronic band structure of the crystal of interest- in this case it is Ge;
- The multiplication table of the O_h^7 space group as it shows explicitly the structure of the group by showing all the possible products of the elements of the O_h^7 space group and
- Standard matrices.

The initial stage in the construction of representations is to commence from a set of linearly independent functions or basis. We then apply an operator $\hat{O}_R$ to each of the elements g of the O_h^7 space group. This process yields a set of n functions $\Psi_1, \Psi_2 \ldots \Psi_n$. If the operator $\hat{O}_R$ now acts on these functions or basis, the outcome can be given as a linear combination of the same n functions[22], that is

$$\hat{O}_{R\psi\nu} = \sum_{\mu=1}^{n} \Psi_{\mu} D_{\mu\nu}(R) \tag{5.18}$$

where $\upsilon = 1, ..., n$.

The matrix representation that corresponds to the element R is $D(R)$. From equation (5.18) and from the equation $\hat{O}_{SR} = \hat{O}_S\hat{O}_R$ we have

$$\hat{O}_{SR\psi\nu} = \hat{O}_S\hat{O}_{R\psi\nu} = \hat{O}_S \sum_{\mu=1}^{n} \Psi_{\mu} D_{\mu\nu}(R) \tag{5.19}$$

$$= \sum_{\mu,\sigma=1}^{n} \Psi_{\sigma} D_{\sigma\mu}(S) D_{\mu\nu}(R)$$

$$= \sum_{\sigma=1}^{n} \Psi_{\sigma} \left[\sum_{\mu=1}^{n} D_{\sigma\mu}(S) D_{\mu\nu}(R) \right]$$

but

$$\hat{O}_{SR\psi\nu} = \sum_{\sigma=1}^{n} \Psi_{\sigma} D_{\sigma\mu}(SR) \tag{5.20}$$

so

$$D_{\mu\nu}(SR) = \sum_{\sigma=1}^{n} D_{\sigma\mu}(S) D_{\mu\nu}(R) \tag{5.21}$$

therefore

$$D(SR) = D(S)D(R) \tag{5.22}$$

A given representation changes its form if we make a different choice of basis, but it is still the same. Two representations that are equivalent may differ because of the choice of basis functions used to express them even though their basic nature is similar. This is where the unitary matrix becomes extremely important. Changing from one basis to another alternates a matrix from R to R'. This is the same as a linear transformation $Y = Ax$. This linear transformation is given by equation (5.23)

$$R^{'} = A'RA \tag{5.23}$$

where $R^{'}$ and R are similar in nature.

The symmetry transformation given by $R^{'} = A'RA$ is a similarity transformation. The diagonal sum or trace or character of a matrix becomes of paramount importance because it is invariant under a similarity transformation. A set of basis functions could be given in terms of x, y, z in space. The basis vectors could also be given in terms of the x, y and z unit vectors. The outcome of a group operation, $\hat{O}_R$, when it operates on a set of basis vectors or alternatively basis functions is a vector or a function which can be expressed as an apt linear combination of the basis vectors or functions . Therefore the group must show invariance under the group symmetry operations.

A group symmetry operation changes basis functions given in terms of (x, y, z) into new functions $(x^{'}, y^{'}, z^{'})$ which are a linear combination of the original functions. The symmetry transformation can be given in various ways that are suitable to the phenomenon and the group representations under consideration. For instance we can have representations of 3×3 matrices acting on a 3-dimensional column vectors. The use of matrix representations are commonly used to denote group representations because non-commutative multiplication is possible and this represents system interaction.

Consider the basis (x, y, z) undergoing a transformation to $(x^{'}, y^{'}, z^{'})$ after being acted upon by group members $g = E, C_6^+, C_3^+, C_3^-, C_2, \ldots$, where g is a symmetry element of the O_h^7 space group. The matrix representation $D(g)$ can be 1×1, $2{\times}2$, $3{\times}3$ etc according to the degeneracy of the irreps of the group or sub-group under consideration. The matrix representation, for instance- for the identity representation, E , can be given in the form depicted by equation 5.24

$$E : \begin{array}{ccc} x^{'} & \rightarrow & x \\ y^{'} & \rightarrow & y \\ z^{'} & \rightarrow & z \end{array} \begin{pmatrix} x^{'} \\ y^{'} \\ z^{'} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{5.24}$$

Likewise the matrix representation for the element C_6^+ is given by

$$C_6^+ : \varphi = \frac{2\pi}{6} = 60^\circ : \begin{array}{ccc} x' & \rightarrow & x+y \\ y' & \rightarrow & -x \\ z' & \rightarrow & z \end{array} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{5.25}$$

Therefore if we consider a basis $\psi_i, i = 1, \ldots, n,$ where $\psi_i = \{\psi_1, \psi_2, \psi_3, ...\}$. We operate on the basis by the symmetry elements of the O_h^7 space group so that it is used to generate all the possible matrix representations of the states of particles or quasi-particles participating in the scattering processes at a given high symmetry point on the BZ. D_{ji} represents the $n \times m$ matrices that can be decomposed or reduced into irreps of smaller dimensions.

The irreducible representations are of paramount importance as they give important information about the system under consideration. Irreducible representations can be viewed as the 'atoms' or building blocks of group representations . A representation of a given dimension is said to be reducible if it can be given as a sum of representations of smaller dimensions that cannot be decomposed to a lower form. For instance, the representation $D_{(g)}^{(3\times3)}$ in equation (5.26)can be decomposed to irreps of lower dimensions.

$$D_{(g)}^{(3\times3)} = D_{(g)}^{(1\times1)} \oplus D_{(g)}^{(2\times2)} \tag{5.26}$$

5.4 Scheme for diagonal and non-diagonal matrix elements

After the derivation of all the matrix representations for the high symmetry points L and Γ we need schemes for diagonal and non-diagonal matrix elements. Consider an electron scattered by a phonon from the Brillouin zone edge, at high symmetry L_3^-, to the zone centre, critical point Γ_{25}^+. This electron- phonon interaction in the valence band of Ge is represented by the Kronecker product hereby stated:

$$\left(L_3^-\right)^{e^-_{initial}} \otimes \left(\Gamma_{25}^+\right)^{e^-_{final}} = L_1^- + L_2^- + 2L_3^-$$

When deriving Clebsch-Gordan coefficients we take the KP that encompass three high symmetry points, for instance from the KP above we have:

$$\left(L_3^-\right)^{2-dim} \otimes \left(\Gamma_{25}^+\right)^{3-dim} \ni \left(L_2^-\right)^{1-dim} \tag{5.27}$$

The product of a 2-dimensional matrix, 3-dimensional matrix and a 1-dimensional matrix gives a 6-dimensional matrix, that is;

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \times \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix} \times c_{11}$$

$$= \begin{bmatrix} a_{11}b_{11}c_{11} & a_{11}b_{12}c_{11} & a_{11}b_{13}c_{11} & a_{12}b_{11}c_{11} & a_{12}b_{12}c_{11} & a_{12}b_{13}c_{11} \\ a_{11}b_{21}c_{11} & a_{11}b_{22}c_{11} & a_{11}b_{23}c_{11} & a_{12}b_{21}c_{11} & a_{12}b_{22}c_{11} & a_{12}b_{23}c_{11} \\ a_{11}b_{31}c_{11} & a_{11}b_{32}c_{11} & a_{11}b_{33}c_{11} & a_{12}b_{31}c_{11} & a_{12}b_{32}c_{11} & a_{12}b_{33}c_{11} \\ a_{21}b_{11}c_{11} & a_{21}b_{12}c_{11} & a_{21}b_{13}c_{11} & a_{22}b_{11}c_{11} & a_{22}b_{12}c_{11} & a_{22}b_{13}c_{11} \\ a_{21}b_{21}c_{11} & a_{21}b_{22}c_{11} & a_{21}b_{23}c_{11} & a_{22}b_{21}c_{11} & a_{22}b_{22}c_{11} & a_{22}b_{23}c_{11} \\ a_{21}b_{31}c_{11} & a_{21}b_{32}c_{11} & a_{21}b_{33}c_{11} & a_{22}b_{31}c_{11} & a_{22}b_{32}c_{11} & a_{22}b_{33}c_{11} \end{bmatrix} \tag{5.28}$$

Using the dimensions and positions of the matrix elements we construct schemes for diagonal and non-diagonal elements of the matrices as depicted by tables 5.1, 5.2, 5.3, 5.4, 5.5, 5.6 and 5.7.

Table 5.1: Clebsch-Gordan coefficients scheme for diagonal matrix elements

Primary Kronecker Product	$\left(L_3^-\right)^{e^-_{initial}} \otimes \left(\Gamma_{25}^+\right)^{e^-_{final}} = L_1^- + L_2^- + 2L_3^-$

Secondary Kronecker Product	$\left(L_3^-\right)^{2-dim} \otimes \left(\Gamma_{25}^+\right)^{3-dim} \ni \left(L_2^-\right)^{1-dim}$		
High Symmetry Points Under Consideration	L_3^-	Γ_{25}^+	L_2^-
Dimension	$2-dim$	$3-dim$	$1-dim$
Diagonal Matrix Elements	11 22	11 22 33	11
Possible Combinations of Matrix Elements Derived from the Diagonal Elements	11	11	11
	11	22	11
	11	33	11
	22	11	11
	22	22	11
	22	33	11

Table 5.2: Clebsch-Gordan coefficients scheme for the first non-diagonal matrix elements derived from the diagonal elements 11 11 11

Primary Kronecker Product	$(L_3^-)^{e^-_{initial}} \otimes (\Gamma_{25}^+)^{e^-_{final}} = L_1^- + L_2^- + 2L_3^-$		
Secondary Kronecker Product	$(L_3^-)^{2-dim} \otimes (\Gamma_{25}^+)^{3-dim} \ni (L_2^-)^{1-dim}$		
High Symmetry Points Under Consideration	L_3^-	Γ_{25}^+	L_2^-
Dimension	$2-dim$	$3-dim$	$1-dim$
Non − diagonal Matrix Elements		11	
	11	21	11
	21	31	
Possible Combinations of Matrix Elements Derived from the Non − diagonal Elements	11	11	11
	11	21	11
	11	31	11
	21	11	11
	21	21	11
	21	31	11

Table 5.3: Clebsch-Gordan coefficients scheme for the second non-diagonal matrix elements derived from the diagonal elements 11 22 11.

Primary Kronecker Product	$\left(L_3^-\right)^{e^-_{initial}} \otimes \left(\Gamma_{25}^+\right)^{e^-_{final}} = L_1^- + L_2^- + 2L_3^-$		
Secondary Kronecker Product	$\left(L_3^-\right)^{2-dim} \otimes \left(\Gamma_{25}^+\right)^{3-dim} \ni \left(L_2^-\right)^{1-dim}$		
High Symmetry Points Under Consideration	L_3^-	Γ_{25}^+	L_2^-
Dimension	$2-dim$	$3-dim$	$1-dim$
Non − diagonal Matrix Elements		12	
	11	22	11
	21	32	
Possible Combinations of Matrix Elements Derived from the Non − diagonal Elements	11	12	11
	11	22	11
	11	32	11
	21	12	11
	21	22	11
	21	32	11

Table 5.4: Clebsch-Gordan coefficients scheme for third non-diagonal matrix elements derived from the diagonal elements 11 33 11.

Primary Kronecker Product	$(L_3^-)^{e^-_{initial}} \otimes (\Gamma_{25}^+)^{e^-_{final}} = L_1^- + L_2^- + 2L_3^-$		
Secondary Kronecker Product	$(L_3^-)^{2-dim} \otimes (\Gamma_{25}^+)^{3-dim} \ni (L_2^-)^{1-dim}$		
High Symmetry Points Under Consideration	L_3^-	Γ_{25}^+	L_2^-
Dimension	$2 - dim$	$3 - dim$	$1 - dim$
Non − diagonal Matrix Elements	11 21	13 23 33	11
Possible Combinations of Matrix Elements Derived from the Non − diagonal Elements	11 11 11 21 21 21	13 23 33 13 23 33	11 11 11 11 11 11

Table 5.5: Clebsch-Gordan coefficients scheme for fourth non-diagonal matrix elements derived from the diagonal elements 22 11 11.

Primary Kronecker Product	$(L_3^-)^{e^-_{initial}} \otimes (\Gamma_{25}^+)^{e^-_{final}} = L_1^- + L_2^- + 2L_3^-$

Secondary Kronecker Product	$(L_3^-)^{2-dim} \otimes (\Gamma_{25}^+)^{3-dim} \ni (L_2^-)^{1-dim}$		
High Symmetry Points Under Consideration	L_3^-	Γ_{25}^+	L_2^-
Dimension	$2-dim$	$3-dim$	$1-dim$
Non – diagonal Matrix Elements	12 22	11 21 31	11
Possible Combinations of Matrix Elements Derived from the Non – diagonal Elements	12 12 12 22 22 22	11 21 31 11 21 31	11 11 11 11 11 11

Table 5.6: Clebsch-Gordan coefficients scheme for the fifth non-diagonal matrix elements derived from the diagonal elements 22 22 11.

Primary Kronecker Product	$(L_3^-)^{e^-_{initial}} \otimes (\Gamma_{25}^+)^{e^-_{final}} = L_1^- + L_2^- + 2L_3^-$		
Secondary Kronecker Product	$(L_3^-)^{2-dim} \otimes (\Gamma_{25}^+)^{3-dim} \ni (L_2^-)^{1-dim}$		
High Symmetry Points Under Consideration	L_3^-	Γ_{25}^+	L_2^-
Dimension	$2-dim$	$3-dim$	$1-dim$
Non − diagonal Matrix Elements	12 22	12 22 32	11
Possible Combinations of Matrix Elements Derived from the Non − diagonal Elements	12	12	11
	12	22	11
	12	32	11
	22	12	11
	22	22	11
	22	32	11

Table 5.7: Clebsch-Gordan coefficients scheme for the sixth non-diagonal matrix elements derived from the diagonal elements 22 33 11.

Primary Kronecker Product	$\left(L_3^-\right)^{e^-_{initial}} \otimes \left(\Gamma_{25}^+\right)^{e^-_{final}} = L_1^- + L_2^- + 2L_3^-$		
Secondary Kronecker Product	$\left(L_3^-\right)^{2-dim} \otimes \left(\Gamma_{25}^+\right)^{3-dim} \ni \left(L_2^-\right)^{1-dim}$		
High Symmetry Points Under Consideration	L_3^-	Γ_{25}^+	L_2^-
Dimension	$2-dim$	$3-dim$	$1-dim$
Non − diagonal Matrix Elements	12 22	13 23 33	11
Possible Combinations of Matrix Elements Derived from the Non − diagonal Elements	12	13	11
	12	23	11
	12	33	11
	22	13	11
	22	23	11
	22	33	11

In order to use the schemes shown by tables 5.1, 5.2, 5.3, 5.4, 5.5, 5.6 and 5.7 we need the matrix representations for the high symmetry points L and Γ. From the secondary Kronecker product under consideration- $\left(L_3^-\right)^{2-dim} \otimes \left(\Gamma_{25}^+\right)^{3-dim} \ni \left(L_2^-\right)^{1-dim}$, the critical symmetry points that are of interest are L_3^-, Γ_{25}^+ and L_2^-. The matrix irreducible representations for these high symmetry points are as as depicted by table 5.8. The group G^{k_Γ} at point Γ has 48 symmetry elements. The sub-group at point L- G^{k_L} has 12 symmetry elements indicated in table 5.8. Using Lagrange's theorem we have

$$\left[G^{k_\Gamma}\right] = n \times \left[G^{k_L}\right] \tag{5.29}$$

where $\left[G^{k_\Gamma}\right]$ refers to the number of elements in the group, G^{k_Γ};

n is an integer and

$\left[G^{k_L}\right]$ is the number of elements in the subgroup G^{k_L}.

Using the theory of coset decomposition, the number of cosets at point L is given by:

$$Number \quad of \quad cosets \quad = \frac{Number \quad of \quad elements \quad in \quad the \quad group \quad G^{k_\Gamma}}{Number \quad of \quad elements \quad in \quad the \quad subgroup \quad G^{k_L}} \tag{5.30}$$

$$= \frac{\left[G^{k_\Gamma}\right]}{\left[G^{k_L}\right]}$$

$$= \frac{48}{12}$$

$$= 4$$

This points to the concept of degeneracy at high symmetry point L. Therefore we have four splittings at the Brillouin zone edge at point L. The matrix representations

Table 5.8: Matrix representations for L_3^-, $\mathit{\Gamma}_{25}^+$ and L_2^- for Ge, O_h^7 space group, for the symmetry elements 1,5,9,13,17 and 21.

High Symmetry Points	O_h^7 *Symmetry Elements*					
	1	5	9	13	17	21
L_3^-	$\begin{matrix}1 & 0\\ 0 & 1\end{matrix}$	$\begin{matrix}\omega^* & 0\\ 0 & \omega^*\end{matrix}$	$\begin{matrix}\omega & 0\\ 0 & \omega^*\end{matrix}$	$\begin{matrix}0 & -1\\ -1 & 0\end{matrix}$	$\begin{matrix}0 & -\omega^*\\ -\omega & 0\end{matrix}$	$\begin{matrix}0 & -\omega\\ -\omega^* & 0\end{matrix}$
Γ_{25}^+	$\begin{matrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{matrix}$	$\begin{matrix}0 & 1 & 0\\ 0 & 0 & 1\\ 1 & 0 & 0\end{matrix}$	$\begin{matrix}0 & 0 & 1\\ 1 & 0 & 0\\ 0 & 1 & 0\end{matrix}$	$\begin{matrix}1 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{matrix}$	$\begin{matrix}0 & 0 & 1\\ 0 & 1 & 0\\ 1 & 0 & 0\end{matrix}$	$\begin{matrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{matrix}$
L_2^-	1	1	1	-1	-1	-1

Table 5.9: Matrix representations for L_3^-, $\mathit{\Gamma}_{25}^+$ and L_2^- for Ge, O_h^7 space group for the symmetry elements 25,29,33,37,41 and 45

High Symmetry Points	O_h^7 *Symmetry Elements*					
	25	29	33	37	41	45
L_3^-	$\begin{matrix}-1 & 0\\ 0 & -1\end{matrix}$	$\begin{matrix}-\omega^* & 0\\ 0 & -\omega\end{matrix}$	$\begin{matrix}-\omega & 0\\ 0 & -\omega^*\end{matrix}$	$\begin{matrix}0 & 1\\ 1 & 0\end{matrix}$	$\begin{matrix}0 & \omega^*\\ \omega & 0\end{matrix}$	$\begin{matrix}0 & \omega\\ \omega^* & 0\end{matrix}$
Γ_{25}^+	$\begin{matrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{matrix}$	$\begin{matrix}0 & 1 & 0\\ 0 & 0 & 1\\ 1 & 0 & 0\end{matrix}$	$\begin{matrix}0 & 0 & 1\\ 1 & 0 & 0\\ 0 & 1 & 0\end{matrix}$	$\begin{matrix}1 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{matrix}$	$\begin{matrix}0 & 0 & 1\\ 0 & 1 & 0\\ 1 & 0 & 0\end{matrix}$	$\begin{matrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{matrix}$
L_2^-	-1	-1	-1	1	1	1

for all the symmetry elements of L_3^- are 2×2 matrices because L_3^- is two-dimensional. For Γ_{25}^+ we use 3×3 matrices because this critical symmetry point is three-dimensional. The same principle is applied to L_2^- which is a one-dimensional high symmetry point.

Using the mathematical theory for the computation of coupling constants [23][24] we determine elements of the unitary matrix or the Clebsch-Gordan coefficients matrix using the equation (5.31)

$$U_{|a|a'|a''}.U^*_{|\bar{a}_0|\bar{a}'_0|\bar{a}''_0} = \frac{dim - d^{k_{l''}}}{[G^{k_L}]} \sum_{x \in G} d^{k_l = \overrightarrow{k}}{}^{L_3^-}(\varphi_x \mid \tau_x)_{a\bar{a}_0} d^{k_{l'} = \overrightarrow{k}}{}^{\Gamma_{25}^+}(\varphi_x \mid \tau_x)_{a'\bar{a}'_0} d^{k_{l''} = \overrightarrow{k}}{}^{L_2^-}(\varphi_x \mid \tau_x)^*_{a''\bar{a}''_0} \tag{5.31}$$

where U is the Clebsch-Gordan coefficients matrix;

U^* is the complex conjugate of the Clebsch-Gordan coefficients matrix;

a, a' and a'' refers to the matrix elements of the irreducible representations l, l' and l'' and these irreps corresponds to the high symmetry points L_3^- ,Γ_{25}^+ and L_2^-;

$dim - d^{k_{l''}}$ refers to the dimensions of L_2^- which is 1 in this case;

$[G^{k_L}]$ is the order of the group G^{k_L} which is 12 in our case;

$k_l = \overrightarrow{k}_{L_3^-}$; $k_{l'} = \overrightarrow{k}_{\Gamma_{25}^+}$and $k_{l''} = \overrightarrow{k}_{L_2^-}$ refers to the wave vectors (momenta $\hbar k$) of the particles or quasi-particles involved in the scattering process- electrons and phonons in our case;

$a\bar{a}_0$, $a'\bar{a}'_0$ and $a''\bar{a}''_0$ gives the positions of the diagonal and non-diagonal matrix elements, for L_3^-, Γ_{25}^+ and L_2^- as shown by table 5.10

Utilising equation (5.31) we hereby present an example of a table that can be used for the derivation of the coupling constants derived from the non-diagonal elements generated from the diagonal elements 22 33 11.

Table 5.10: Example of table of derivation of coupling constants for Ge, space group O_h^7, derived from the non-diagonal matrix elements generated from the diagonal elements 22 33 11 for symmetry elements 1,5,9,13,17,21 and 25.

Matrix Elements Positions	O_h^7 *Symmetry Elements*						
L_3^- Γ_{25}^+ L_2^- $a\bar{a}_0$ $a'\bar{a}'_0$ $a''\bar{a}''_0$	1	5	9	13	17	21	25
12 13 11	$\frac{1}{12}\{[1.0.1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$
12 23 11	$\frac{1}{12}\{[1.0.1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$
12 33 11	$\frac{1}{12}\{[0.1.1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$
22 13 11	$\frac{1}{12}\{[1.0.1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$
22 23 11	$\frac{1}{12}\{[1.0.1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$
22 33 11	$\frac{1}{12}\{[1.1.1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$	$[..]+$

(a) Example of table of derivation of coupling constants for Ge, space group O_h^7, derived from the non-diagonal matrix elements generated from the diagonal elements 22 33 11 for symmetry elements 29,33,37,41 and 45.

Matrix Elements Positions	O_h^7 *Symmetry Elements*					U^2
L_3^- Γ_{25}^+ L_2^- $a\bar{a}_0$ $a'\bar{a}'_0$ $a''\bar{a}''_0$	29	33	37	41	45	
12 13 11	$+[0.0.-1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[\omega.0.1^*]\}$	$=\frac{\omega^*}{6}$
12 23 11	$+[0.1.-1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[\omega.0.1^*]\}$	$=\frac{1}{6}$
12 33 11	$+[0.0.-1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[\omega.1.1^*]\}$	$=\frac{\omega}{6}$
22 13 11	$+[-\omega.0.-1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[0.0.1^*]\}$	$=\frac{\omega}{6}$
22 23 11	$+[-\omega.1.-1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[0.0.1^*]\}$	$=\frac{\omega}{6}$
22 33 11	$+[-\omega.0.-1^*]$	$+[..]+$	$[..]+$	$[..]+$	$[0.1.1^*]\}$	$=\frac{1}{6}$

Using the calculated values of the square of the elements of the U-matrix as depicted in the table 5.10a, we hereby present the Clebsch-Gordan coefficients for the blocks $U_{111}, U_{121}, U_{131}, U_{211}, U_{221}$ and U_{231}.

$$|U^2_{12\quad 13\quad 11}| = \frac{\omega^*}{6} \Longrightarrow U_{12\quad 13\quad 11} = \pm\sqrt{\frac{\omega^*}{6}} \tag{5.32}$$

$$|U^2_{12\quad 23\quad 11}| = \frac{1}{6} \Longrightarrow U_{12\quad 23\quad 11} = \pm\sqrt{\frac{1}{6}} \tag{5.33}$$

$$|U^2_{12\quad 33\quad 11}| = \frac{\omega}{6} \Longrightarrow U_{12\quad 33\quad 11} = \pm\sqrt{\frac{\omega}{6}} \tag{5.34}$$

$$|U^2_{22\quad 13\quad 11}| = \frac{\omega^*}{6} \Longrightarrow U_{22\quad 13\quad 11} = \pm\sqrt{\frac{\omega^*}{6}} \tag{5.35}$$

$$|U^2_{22\quad 23\quad 11}| = \frac{\omega}{6} \Longrightarrow U_{22\quad 23\quad 11} = \pm\sqrt{\frac{\omega}{6}} \tag{5.36}$$

$$|U^2_{22\quad 33\quad 11}| = \frac{1}{6} \Longrightarrow U_{22\quad 33\quad 11} = \pm\sqrt{\frac{1}{6}} \tag{5.37}$$

The six different blocks and their respective Clebsch-Gordan coefficients are:

$$U_{111} = \pm\sqrt{\frac{\omega^*}{6}}$$

$$U_{121} = \pm\sqrt{\frac{1}{6}}$$

$$U_{131} = \pm\sqrt{\frac{\omega}{6}}$$

$$U_{211} = \pm\sqrt{\frac{\omega^*}{6}}$$

$$U_{221} = \pm\sqrt{\frac{\omega}{6}}$$

$$U_{231} = \pm\sqrt{\frac{1}{6}}$$

The same procedure was done for all the non-diagonal elements that yielded the coupling constants shown in tables 6.1, 6.2, 6.3 and 6.4.

Chapter 6

Results and Discussion

In this chapter we present the derived Clebsch-Gordan coefficients that are utilised in the interpretation of the electron-phonon scattering process within the valence band of Ge. We use the calculated coupling constants and the experimental evidence to comprehend the phenomenon that happens when electrons are scattered by phonons from the Brilloun zone edge, at the critical point L_3^-, to the zone centre at high symmetry point-Γ_{25}^+.

6.1 Results

We hereby present the calculated Clebsch-Gordan coefficients in tabular form for clarity purpose. For the secondary Kronecker products $L_3^- \otimes \Gamma_{25}^+ \ni L_2^-$and $L_3^- \otimes \Gamma_{25}^+ \ni L_1^-$, the blocks under consideration are U$_{111}$,U$_{121}$,U$_{131}$,U$_{211}$,U$_{221}$ and U_{231}. We derived these coupling constants from six different types of non-diagonal matrix elements. The last columns of table 6.1 and table 6.2 shows the outcomes of the summation of the U-matrix and its complex conjugate U^*. This yielded a 0 for the two respective cases. Tables 6.3 and 6.4 shows the calculated Clebsch-Gordan coefficients for the secondary Kronecker product $L_3^- \otimes \Gamma_{25}^+ \ni L_3^-$. The coupling constants are derived from twelve different types of non-diagonal matrix elements. In this case the blocks under consideration are of two types, that is $U_{111}, U_{121}, U_{131}, U_{211}, U_{221}, U_{231}$ and $U_{112}, U_{122}, U_{132}, U_{212}, U_{222}, U_{232}$. The summation of the U- matrix and its complex conjugate U^*yielded a 0 and a 1 for some

Table 6.1: Clebsch-Gordan coefficients for the Kronecker product $L_3^- \otimes \Gamma_{25}^+ \ni L_2^-$ for Ge, O_h^7 space group.

$Block$	$Clebsch-$ $Gordan$ $Coefficients$ $from$ $Non-diagonal$ $Elements$						$\sum UU^*$
	1^{st}	2^{nd}	3^{rd}	4^{th}	5^{th}	6^{th}	
U_{111}	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{\omega}{6}}$	0
U_{121}	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	0
U_{131}	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{1}{6}}$	0
U_{211}	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{\omega}{6}}$	0
U_{221}	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{1}{6}}$	0
U_{231}	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	0

blocks as depicted in tables 6.3 and 6.4.

Table 6.2: Clebsch-Gordan coefficients for the Kronecker product $L_3^- \otimes \Gamma_{25}^+ \ni L_1^-$ for Ge, O_h^7 space group.

	$Clebsch-Gordan\ Coefficients\ from\ Non-diagonal\ Elements$						
$Block$	1^{st}	2^{nd}	3^{rd}	4^{th}	5^{th}	6^{th}	$\sum UU^*$
U_{111}	$i\sqrt{\frac{1}{6}}$	$i\sqrt{\frac{\omega}{6}}$	$i\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{\omega}{6}}$	0
U_{121}	$i\sqrt{\frac{\omega}{6}}$	$i\sqrt{\frac{\omega^*}{6}}$	$i\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	0
U_{131}	$i\sqrt{\frac{\omega^*}{6}}$	$i\sqrt{\frac{1}{6}}$	$i\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{1}{6}}$	0
U_{211}	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$i\sqrt{\frac{1}{6}}$	$i\sqrt{\frac{\omega^*}{6}}$	$i\sqrt{\frac{\omega}{6}}$	0
U_{221}	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{1}{6}}$	$\sqrt{\frac{\omega}{6}}$	$i\sqrt{\frac{\omega^*}{6}}$	$i\sqrt{\frac{\omega}{6}}$	$i\sqrt{\frac{1}{6}}$	0
U_{231}	$\sqrt{\frac{\omega}{6}}$	$\sqrt{\frac{\omega^*}{6}}$	$\sqrt{\frac{1}{6}}$	$i\sqrt{\frac{\omega}{6}}$	$i\sqrt{\frac{1}{6}}$	$i\sqrt{\frac{\omega^*}{6}}$	0

Table 6.3: Clebsch-Gordan coefficients for the Kronecker product $L_3^- \otimes \Gamma_{25}^+ \ni L_3^-$ for Ge, O_h^7 space group [blocks U_{111},U_{121},U_{131},U_{211},U_{221} and U_{231}]

$Block$	1^{st}	2^{nd}	3^{rd}	4^{th}	5^{th}	6^{th}	7^{th}	8^{th}	9^{th}	10^{th}	11^{th}	12^{th}	$\sum UU^*$
U_{111}	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	1
U_{121}	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	1
U_{131}	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	1
U_{211}	0	$\frac{1}{\sqrt{3}}$	0	$\sqrt{\frac{\omega}{3}}$	0	$\sqrt{\frac{\omega^*}{3}}$	$\frac{1}{\sqrt{3}}$	0	$\sqrt{\frac{\omega^*}{3}}$	0	$\sqrt{\frac{\omega}{3}}$	0	0
U_{221}	0	$\sqrt{\frac{\omega}{3}}$	0	$\sqrt{\frac{\omega^*}{3}}$	0	$\frac{1}{\sqrt{3}}$	$\sqrt{\frac{\omega}{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\sqrt{\frac{\omega^*}{3}}$	0	0
U_{231}	0	$\sqrt{\frac{\omega^*}{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\sqrt{\frac{\omega}{3}}$	$\sqrt{\frac{\omega^*}{3}}$	0	$\sqrt{\frac{\omega}{3}}$	0	$\frac{1}{\sqrt{3}}$	0	0

Table 6.4: Clebsch-Gordan coefficients for the Kronecker product $L_3^- \otimes \Gamma_{25}^+ \ni L_3^-$ for Ge, O_h^7 space group [blocks U_{112},U_{122},U_{132},U_{212},U_{222} and U_{232}]

$Block$	1^{st}	2^{nd}	3^{rd}	4^{th}	5^{th}	6^{th}	7^{th}	8^{th}	9^{th}	10^{th}	11^{th}	12^{th}	$\sum UU^*$
U_{112}	0	$\frac{1}{\sqrt{3}}$	0	$\sqrt{\frac{\omega}{3}}$	0	$\sqrt{\frac{\omega^*}{3}}$	$\frac{1}{\sqrt{3}}$	0	$\sqrt{\frac{\omega^*}{3}}$	0	$\sqrt{\frac{\omega}{3}}$	0	0
U_{122}	0	$\sqrt{\frac{\omega^*}{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\sqrt{\frac{\omega}{3}}$	$\sqrt{\frac{\omega^*}{3}}$	0	$\sqrt{\frac{\omega}{3}}$	0	$\frac{1}{\sqrt{3}}$	0	0
U_{132}	0	$\sqrt{\frac{\omega}{3}}$	0	$\sqrt{\frac{\omega^*}{3}}$	0	$\frac{1}{\sqrt{3}}$	$\sqrt{\frac{\omega}{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\sqrt{\frac{\omega^*}{3}}$	0	0
U_{212}	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	1
U_{222}	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	1
U_{232}	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	0	$\frac{1}{\sqrt{3}}$	1

6.2 Discussion of results

The dynamics of a quasi-particle or a particle is explained using the wave function- ψ. The wave function has the possible information of the system that can be measured. The wave function cannot be measured directly because it is a true complex function. In order to get a real value we have to measure its intensity which is given by

$$\psi(\vec{r},t)\psi(\vec{r},t)^{*} = |\psi(\vec{r},t)|^{2} \tag{6.1}$$

This intensity is a measure of the particle's presence in a space under considerations. The likelihood of finding the particle is directly proportional to $|\psi(r,t)\ |^{2}$[25]. If we are certain that the particle is definitely in a given space, we normalise the intensity, $|\psi(\vec{r},t)\ |\ ^{2}$, so that integration perfomed over all space yields a unity, that is

$$\int_{-\infty}^{+\infty} [\psi(\vec{r},t)\psi(\vec{r},t)^{*}] = 1 \tag{6.2}$$

The above equation represents the probability of finding the system under consideration at a particular position and time. Group theoretically, we can use the U-matrix or Clebsch-Gordan coefficients matrix to derive the same information. Our results shows that the summation of the U-matrix and its complex conjugate U^{*} either gives a zero or a one, ie

$$\sum UU^{*} = |U|^{2} = 1 \tag{6.3}$$

$$\sum UU^{*} = |U|^{2} = 0 \tag{6.4}$$

For the Kronecker product $L_{3}^{-} \otimes \Gamma_{25}^{+} \ni L_{1}^{-}$, the summation of the product of the U-matrix and its complex conjugate, U^{*}, gives a zero for all the blocks. This implies that the type of phonon represented by L_{1}^{-} is not allowed to take part in that transition. Group theoretically, this means that the phonon type denoted by L_{1}^{-} is not contained in the product representation $L_3^- \otimes \Gamma_{25}^+$.

Likewise, for the Kronecker product $L_3^- \otimes \Gamma_{25}^+ \ni L_2^-$, the summation of the product of the U-matrix and its complex conjugate U^*, yields a zero for all the blocks. Therefore according to my calculations L_2^- is not contained in the product $L_3^- \otimes \Gamma_{25}^+$. This means that the phonon represented by L_2^- does not take part in the transition.

However, for the Kronecker product $L_3^- \otimes \Gamma_{25}^+ \ni L_3^-$, the summation of the product of the U-matrix and its complex conjugate, U^*, yields a one for some blocks, that is $\sum UU^* = |U|^2 = 1$ Therefore, the phonon type represented by L_3^- is allowed to take part in this transition. The calculated Clebsch-Gordan coefficients belongs to two types of blocks, i.e $U_{111}, U_{121}, U_{131}, U_{211}, U_{221}, U_{231}$ and $U_{112}, U_{122}, U_{132}, U_{212}, U_{222}, U_{232}$. This depicts degeneracy at the high symmetry point L_3^-, hence we have the L_3^- symmetry of two kinds and this is consistent with the Kronecker product $\left(L_3^-\right)^{e^-_{initial}} \otimes \left(\Gamma_{25}^+\right)^{e^-_{final}} = L_1^- + L_2^- + 2L_3^-$. The experimentally obtained phonon dispersion curve of Ge[14] shows the types of phonons allowed to take part in the transition of carriers in the valence and conduction bands of Ge.

The vibration spectrum of Ge as depicted by figure 6.1 taken from [3], shows that L_2^- represents the LA phonon, L_3^- represents the TO phonon and L_1^- symmetry is completely absent. According to Lax and Hopfield[17], in the valence band the electron-phonon transition is represented by the Kronecker product hereby stated,

$$L_3^- \otimes \Gamma_{25}^+ = L_1^- + L_2^- + 2L_3^-$$

which implies that

$$L_3^- \otimes \Gamma_{25}^+ = none + LA + 2TO \tag{6.5}$$

However my calculations shows that for the electron-phonon transition from L_3^- to Γ_{25}^+ , the LA phonon doesn't take part although it is present in some transitions in the valence band of Ge. It is only the TO phonons that take part in this transition. Therefore the Kronecker product has to be modified to equation (6.6), ie

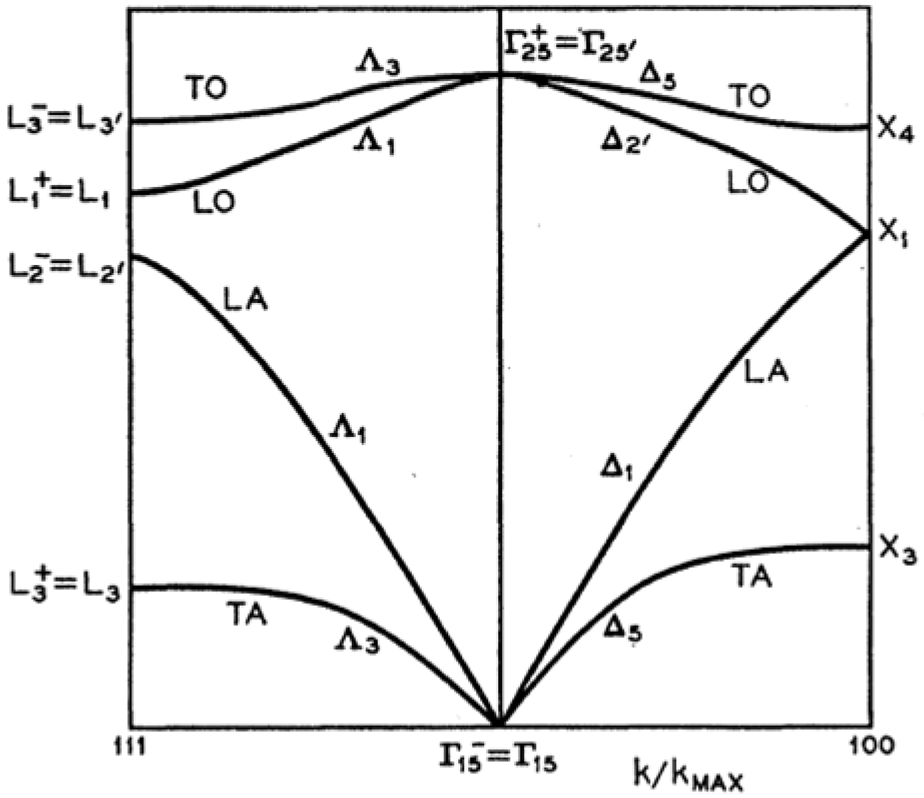


Figure 6.1: The vibration spectrum for Ge [14].

$$L_3^- \otimes \Gamma_{25}^+ = L_1^- + L_2^- + 2L_3^-$$

which implies that

$$L_3^- \otimes \Gamma_{25}^+ = none + none + 2TO \tag{6.6}$$

Analysis of the phonon dispersion curves obtained by Brockhouse and Iyengar[14] shows that our theoretical results are consistent with the experimental outcome which shows that it is only the transverse optical phonons that participate in the scattering of electrons from the Brillouin zone edge at point $L_3^-$to the zone centre at point Γ_{25}^+. The phonon dipersion curve as depicted by figure 6.1 is in good agreement with our theoretical outcome as shown by equation (6.6). We have therefore modified equation (6.5) which is given as such in the article by Lax and Hopfield[17].

Chapter 7

Conclusion

Using group theoretical techniques, we have calculated Clebsch-Gordan coefficients that are used to interpret the scattering of electrons by phonons from the Brillouin zone edge of germanium $\left(O_h^7\right)$ at the high symmetry point L_3^- to the zone centre at high symmetry point Γ_{25}^+. Using the computed coupling constants we also found out that when electrons are scattered by phonons from the Brillouin zone edge at high symmetry point L_3^- to the zone centre at point Γ_{25}^+ within the valence band of Ge, both the LA and TO phonons are present but only the TO phonons participate in the scattering process. The LO phonons are completely absent for these types of transitions in the valence band of Ge. Our findings are consistent with the vibration spectrum for Ge experimentally obtained by Brockhouse and Iyenger[14].

We explicitly showed that the Clebsch-Gordan coefficients are computed from the non-diagonal matrix elements. It is therefore the non-diagonal matrix elements that carry the essential information. We have also deduced that the summation of the product of the U-matrix and its complex conjugate, U^*, either gives a 0 or a 1 for different blocks under consideration, i.e

$$\sum UU^* = |U|^2 = 1$$

or

$$\sum UU^* = |U|^2 = 0$$

Table 7.1: Types of phonons and symmetry assignments for scattering of electrons from L_3^- to Γ_{25}^+ in the valence band of Ge for the Kronecker product $L_3^- \otimes \Gamma_{25}^+ = L_1^- + L_2^- + 2L_3^-$

Phonon Type	*Sym Assign*	*Presence in Ge VB*	*Partcipation in scattering of electrons from* L_3^- *to* Γ_{25}^+ *in Ge VB*	$\sum UU^*$
TO	L_3^-	$\surd$	$\surd$	1 *for some blocks*
LA	L_2^-	$\surd$	$\times$	0 *for all blocks*
LO	L_1^-	$\times$	$\times$	0 *for all blocks*

We have interpreted this to mean that the perturbation factor is either allowed to take part in the transition or forbidden. In our case the pertubation factor are the phonons. Table 7.1 is a summary of our group theoretical outcomes.

Our results can be applicable to similar semiconductors such as silicon. As outlined in the introductory chapter of this dissertation we can conclude that the objectives of this work have been met.

7.1 Future work

The possibility of using Clebsch-Gordan coefficients to describe scattering processes in doped crystals is an area that may be of interest. Moreover the possibility of utilising Clebsch-Gordan coefficients to determine the strength of electron-phonon scattering in various channel directions in the Brillouin zone of germanium and similar crystals is an area that still needs to be explored. The role played by electron-phonon scattering in the physics of quantum dots, nano-structures and the field of lasers provide interesting ground for future work.

Appendix A

Irreps at the L-point for O_h^7 space group

The group G^{k_L} is a subgroup of the group G^{k_Γ}. The high symmetry points at L are $L_{1\pm}$, $L_{2\pm}$, $L_{3\pm}$, $L_{4\pm}$, $L_{5\pm}$ and $L_{6\pm}$ .At the high symmetry point L we have 12 symmetry elements, that is 1, 5, 9, 13, 17, 21, 25, 29, 33, 37, 41 and 45. In order to generate the matrix representations for all the symmetry elements at point L we use generators or augumenters. The generators at L are the symmetry elements 9, 13 and 37. For instance, using the O_h^7 multiplication table as shown in appendix E we can generate the matrix representations for the symmetry elements 5 and 17 by $9{\times}9 = 5$ and $13{\times}9 = 17$ respectively. Using the O_h^7 combination table, all the matrix irreducible representations at the L point are generated.

Table A.1: Irreducible representations for the high symmetry point L, O_h^7 space group, for symmetry elements 1,5,9,13,17 and 21.

L	*Identity*	$9 \times 9 = 5$	*Gen*	*Gen*	$13 \times 9 = 17$	$9 \times 13 = 69(21)$
Sym Ele	1	5	9	13	17	21
L_1^+	1	1	1	1	1	1
L_1^-	1	1	1	1	1	1
L_2^+	1	1	1	-1	-1	-1
L_2^-	1	1	1	-1	-1	-1
L_3^+	$\begin{matrix}1 & 0\\ 0 & 1\end{matrix}$	$\begin{matrix}\omega^* & 0\\ 0 & \omega\end{matrix}$	$\begin{matrix}\omega & 0\\ 0 & \omega^*\end{matrix}$	$\begin{matrix}0 & 1\\ 1 & 0\end{matrix}$	$\begin{matrix}0 & \omega^*\\ \omega & 0\end{matrix}$	$\begin{matrix}0 & \omega\\ \omega^* & 0\end{matrix}$
L_3^-	$\begin{matrix}1 & 0\\ 0 & 1\end{matrix}$	$\begin{matrix}\omega^* & 0\\ 0 & \omega\end{matrix}$	$\begin{matrix}\omega & 0\\ 0 & \omega^*\end{matrix}$	$\begin{matrix}0 & -1\\ -1 & 0\end{matrix}$	$\begin{matrix}0 & -\omega^*\\ -\omega & 0\end{matrix}$	$\begin{matrix}0 & -\omega\\ -\omega^* & 0\end{matrix}$
L_4^+	1	1	-1	i	$-i$	i
L_4^-	1	1	-1	i	$-i$	i
L_5^+	1	1	-1	$-i$	i	$-i$
L_5^-	1	1	-1	$-i$	i	$-i$
L_6^+	$\begin{matrix}1 & 0\\ 0 & 1\end{matrix}$	$\begin{matrix}\omega & 0\\ 0 & \omega^*\end{matrix}$	$\begin{matrix}-\omega^* & 0\\ 0 & -\omega\end{matrix}$	$\begin{matrix}0 & 1\\ -1 & 0\end{matrix}$	$\begin{matrix}0 & -\omega\\ \omega^* & 0\end{matrix}$	$\begin{matrix}0 & \omega^*\\ -\omega & 0\end{matrix}$
L_6^-	$\begin{matrix}1 & 0\\ 0 & 1\end{matrix}$	$\begin{matrix}\omega & 0\\ 0 & \omega^*\end{matrix}$	$\begin{matrix}-\omega^* & 0\\ 0 & -\omega\end{matrix}$	$\begin{matrix}0 & -1\\ 1 & 0\end{matrix}$	$\begin{matrix}0 & \omega\\ -\omega^* & 0\end{matrix}$	$\begin{matrix}0 & -\omega^*\\ \omega & 0\end{matrix}$

(a) Irreducible representations for the high symmetry point L, O_h^7 space group, for symmetry elements 25,29,33,37,41 and 45.

L	$5 \times 33 = 73$	$37 \times 21 = 77$	$21 \times 37 = 33$	*Gen*	$37 \times 9 = 41$	37×5
Sym Ele	25	29	33	37	41	45
L_1^+	1	1	1	1	1	1
L_1^-	-1	-1	-1	-1	-1	-1
L_2^+	1	1	1	-1	-1	-1
L_2^-	-1	-1	-1	1	1	1
L_3^+	$\begin{matrix}1 & 0\\ 0 & 1\end{matrix}$	$\begin{matrix}\omega^* & 0\\ 0 & \omega\end{matrix}$	$\begin{matrix}\omega & 0\\ 0 & \omega^*\end{matrix}$	$\begin{matrix}0 & 1\\ 1 & 0\end{matrix}$	$\begin{matrix}0 & \omega^*\\ \omega & 0\end{matrix}$	$\begin{matrix}0 & \omega\\ \omega^* & 0\end{matrix}$
L_3^-	$\begin{matrix}-1 & 0\\ 0 & -1\end{matrix}$	$\begin{matrix}-\omega^* & 0\\ 0 & -\omega\end{matrix}$	$\begin{matrix}-\omega & 0\\ 0 & -\omega^*\end{matrix}$	$\begin{matrix}0 & 1\\ 1 & 0\end{matrix}$	$\begin{matrix}0 & \omega^*\\ \omega & 0\end{matrix}$	$\begin{matrix}0 & \omega\\ \omega^* & 0\end{matrix}$
L_4^+	1	1	-1	i	$-i$	i
L_4^-	-1	-1	1	$-i$	i	$-i$
L_5^+	1	1	-1	$-i$	i	$-i$
L_5^-	-1	-1	1	i	-i	i
L_6^+	$\begin{matrix}1 & 0\\ 0 & 1\end{matrix}$	$\begin{matrix}\omega & 0\\ 0 & \omega^*\end{matrix}$	$\begin{matrix}-\omega^* & 0\\ 0 & -\omega\end{matrix}$	$\begin{matrix}0 & 1\\ -1 & 0\end{matrix}$	$\begin{matrix}0 & -\omega\\ \omega^* & 0\end{matrix}$	$\begin{matrix}0 & \omega^*\\ -\omega & 0\end{matrix}$
L_6^-	$\begin{matrix}-1 & 0\\ 0 & -1\end{matrix}$	$\begin{matrix}-\omega & 0\\ 0 & -\omega^*\end{matrix}$	$\begin{matrix}\omega^* & 0\\ 0 & \omega\end{matrix}$	$\begin{matrix}0 & 1\\ -1 & 0\end{matrix}$	$\begin{matrix}0 & -\omega\\ \omega^* & 0\end{matrix}$	$\begin{matrix}0 & \omega^*\\ -\omega & 0\end{matrix}$

Appendix B

Irreps at Γ-point for O_h^7 space group

The group of symmetry elements at the Γ-point, G^{k_Γ} is the main group in the first Brillouin zone of the O_h^7 space group. At this high symmetry point we have 48 symmetry elements. The generators or augumenters in a group as shown by table B.1 act like basis vectors in a vector space. The basis vectors span a vector space and generate all the vector space elements. The generators span a group and generate all the representations for the group elements. At the Γ-point the critical symmetry points that we are considering are $\Gamma_{1\pm}$, $\Gamma_{2\pm}$, $\Gamma_{3\pm}$, $\Gamma_{4\pm}$ and $\Gamma_{5\pm}$.

Table B.1: Irreducible representations at the Brillioun zone centre- Γ-point, for O_h^7 space group for symmetry elements 1,5,9,13,17 and 21

Γ	*Ident*	$9 \times 9 = 5$	*Gen*	$37 \times 25 = 13$	$13 \times 9 = 17$	$9 \times 13 = 2\bar{1}$
	1	5	9	13	17	21
Γ_1^+	1	1	1	1	1	1
Γ_1^-	1	1	1	1	1	1
Γ_2^+	1	1	1	-1	-1	-1
Γ_2^-	1	1	1	-1	-1	-1
Γ_3^+	$\begin{matrix} 1 & 0 \\ 0 & 1 \end{matrix}$	$\begin{matrix} \omega^* & 0 \\ 0 & \omega \end{matrix}$	$\begin{matrix} \omega & 0 \\ 0 & \omega^* \end{matrix}$	$\begin{matrix} 0 & 1 \\ 1 & 0 \end{matrix}$	$\begin{matrix} 0 & \omega^* \\ \omega & 0 \end{matrix}$	$\begin{matrix} 0 & \omega \\ \omega^* & 0 \end{matrix}$
Γ_3^-	$\begin{matrix} 1 & 0 \\ 0 & 1 \end{matrix}$	$\begin{matrix} \omega^* & 0 \\ 0 & \omega \end{matrix}$	$\begin{matrix} \omega & 0 \\ 0 & \omega^* \end{matrix}$	$\begin{matrix} 0 & -1 \\ -1 & 0 \end{matrix}$	$\begin{matrix} 0 & -\omega^* \\ -\omega & 0 \end{matrix}$	$\begin{matrix} 0 & -\omega \\ -\omega^* & 0 \end{matrix}$
Γ_4^+	$\begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{matrix}$
Γ_4^-	$\begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{matrix}$
Γ_5^+	$\begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{matrix}$
Γ_5^-	$\begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{matrix}$

(a) Irreducible representations at the Brillioun zone centre- Γ-point, for O_h^7 space group for symmetry elements 25,29,33,37,41 and 45.

25	$37 \times 21 = 29$	$21 \times 37 = 33$	*Gen*	$37 \times 9 = 41$	$37 \times 5 = 45$
25	29	33	37	41	45
1	1	1	1	1	1
-1	-1	-1	-1	-1	-1
1	1	1	-1	-1	-1
-1	-1	-1	1	1	1
I	$\begin{matrix} \omega^* & 0 \\ 0 & \omega \end{matrix}$	$\begin{matrix} \omega & 0 \\ 0 & \omega^* \end{matrix}$	$\begin{matrix} 0 & 1 \\ 1 & 0 \end{matrix}$	$\begin{matrix} 0 & \omega^* \\ \omega & 0 \end{matrix}$	$\begin{matrix} 0 & \omega \\ \omega^* & 0 \end{matrix}$
$-I$	$\begin{matrix} -\omega^* & 0 \\ 0 & -\omega \end{matrix}$	$\begin{matrix} -\omega & 0 \\ 0 & -\omega^* \end{matrix}$	$\begin{matrix} 0 & 1 \\ 1 & 0 \end{matrix}$	$\begin{matrix} 0 & \omega^* \\ \omega & 0 \end{matrix}$	$\begin{matrix} 0 & \omega \\ \omega^* & 0 \end{matrix}$
I	$\begin{matrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix}$	$-\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$	- $\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$	- $\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
$-I$	$-\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$	$-\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$	$\begin{matrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{matrix}$
I	$\begin{matrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{matrix}$	$\begin{matrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{matrix}$	$\begin{matrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{matrix}$
$-I$	$-\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$	$-\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$	$-\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$	- $\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$	$-\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

Appendix C

Irreps labeling at the BZ centre for O_h^7 group

The labelling of the critical symmetry points varies even though we are dealing with the same high symmetry points on a given Brillouin zone. We hereby present the equivalent labelling of irreducible representations at the Brillouin zone centre at point Γ as depicted by table C.1[9],[10],[11].

Table C.1: Equivalent labeling of irreducible representations at high symmetry point Γ, for O_h^7 space group [9, 10, 11]

CDML	Miller, Love	Zak, Casher	Kovalev	BC	Elliot	BSW
Γ_{1+}	GM1+	1	T2005_{τ_1}	A_{1g}	Γ_{+}	Γ_1
Γ_{2+}	GM2+	2	T2005_{τ_2}	A_{2g}	Γ_{2+}	Γ_2
Γ_{3+}	GM3+	3	T2005_{τ_3}	E_g	Γ_{12+}	Γ_{12}
Γ_{4+}	GM4+	5	T2005_{τ_5}	T_{1g}	Γ_{15+}	$\Gamma_{15'}$
Γ_{5+}	GM5+	4	T2005_{τ_4}	T_{2g}	Γ_{25+}	$\Gamma_{25'}$
Γ_{1-}	GM1-	6	T2005_{τ_6}	A_{1u}	Γ_{1-}	$\Gamma_{1'}$
Γ_{2-}	GM2-	7	T2005_{τ_7}	A_{2u}	Γ_{2-}	$\Gamma_{2'}$
Γ_{3-}	GM3-	8	T2005_{τ_8}	E_u	Γ_{12-}	$\Gamma_{12'}$
Γ_{4-}	GM4-	10	$\text{T2005}_{\tau_{10}}$	T_{1u}	Γ_{15-}	Γ_{15}
Γ_{5-}	GM5-	9	T2005_{τ_9}	T_{2u}	Γ_{25-}	Γ_{25}
Γ_{6+}	GM6+	$\bar{1}$	P205_{π_2}	$\bar{E}_{1g}$	Γ_{6+}	_
Γ_{7+}	GM7+	$\bar{2}$	P205_{π_1}	$\bar{E}_{2g}$	Γ_{7+}	_
Γ_{8+}	GM8+	$\bar{3}$	P205_{π_3}	$\bar{F}_g$	Γ_{8+}	_
Γ_{6-}	GM6-	$\bar{4}$	P205_{π_4}	$\bar{E}_{1u}$	Γ_{6-}	_
Γ_{7-}	GM7-	$\bar{5}$	P205_{π_5}	$\bar{E}_{2u}$	Γ_{7-}	_
Γ_{8-}	GM8-	$\bar{6}$	P205_{π_6}	$\bar{F}_u$	Γ_{8-}	_

Appendix D

BZ points and coordinates for O_h^7 space group

The critical symmetry points have coordinates that we use to locate their positions on the Brillouin zone. Table D.1 shows the coordinates for the high symmetry points and lines for the first Brillouin zone of the O_h^7 space group[11].

Table D.1: Lines, high symmetry points and their coordinates and single valued irreducible representations for O_h^7 space group [11].

Points and Lines	Cordinates	Single-valued Irreducible representations
Γ	$(0,0,0)$	$\Gamma_{1\pm,2\pm,3\pm,4\pm,5\pm}$
X	$\left(\frac{1}{2},0,\frac{1}{2}\right)$	$X_{1,2,3,4}\,(2)\,R-Reps$
L	$\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$	$L_{1\pm,2\pm}\,(1)$,$L_{3\pm}\,(2)\,R-Reps$
W	$\left(\frac{1}{2},\frac{1}{4},\frac{3}{4}\right)$	$W_{1,2}\,(2)\,C-Reps$
Δ	$(\alpha,0,\alpha)$	$\Delta_{1,2,3,4}\,(1)\,,\Delta_5\,(2)\,C-Reps$
$\mathit{\Lambda}$	(α,α,α)	$\mathit{\Lambda}_{1,2}\,(1)\,,\mathit{\Lambda}_3\,(2)\,R-Reps$
Σ	$(\alpha,\alpha,2\alpha)$	$\Sigma_{1,2,3,4}\,(1)\,C-Reps$
Q	$\left(\frac{1}{2},\frac{1}{4}+\alpha,\frac{3}{4}+\alpha\right)$	$Q_{1,2}\,(1)\,R-Reps$
S	$\left(\frac{1}{2}+\alpha,2\alpha,\frac{1}{2}+\alpha\right)$	$S_{1,2,3,4}\,(1)\,R-Reps$
A	$(\alpha,-\alpha+\beta,\beta)$	$A_{1,2}\,(1)\,C-Reps$
$Z=V$	$\left(\frac{1}{2},\alpha,\frac{1}{2}+\alpha\right)$	$Z_1=V_1\,(2)\,R-Reps$

Appendix E

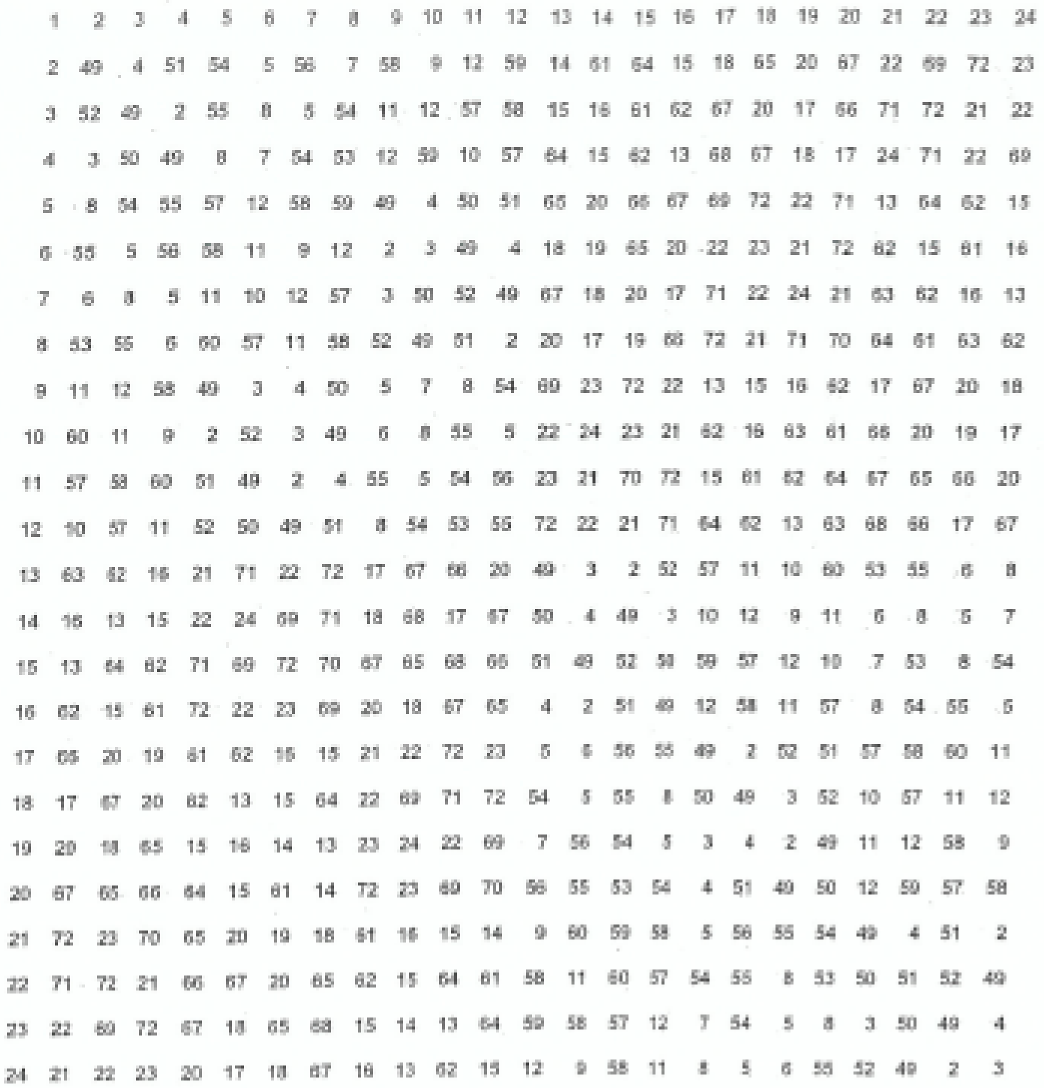
Multiplication table for O_h^7 space group

The germanium space group has 48 by 48 symmetry elements. The possible combinations of all the elements give us a huge multiplication table. In order to simplify this multiplication table we have divided it into 16 components that have to be arranged correctly when using the O_h^7 combination table. The scheme below gives the correct arrangement of the 16 components of the O_h^7, multiplication table.

Table E.1: Scheme for the arrangement of the 16 components of the multiplication table for O_h^7 space group

O_h^7 *Sym Elem*	$1, 2, 3, 4, 5$..........	....	....	.........,$93, 94, 95, 96$
1 2 3 4 5 . . . . 92 93 94 95 96	Component No 1	Component No 2	Component No 3	Component No 4
	Component No 5	Component No 6	Component No 7	Component No 8
	Component No 9	Component No 10	Component No 11	Component No 12
	Component No 13	Component No 14	Component No 15	Component No 16

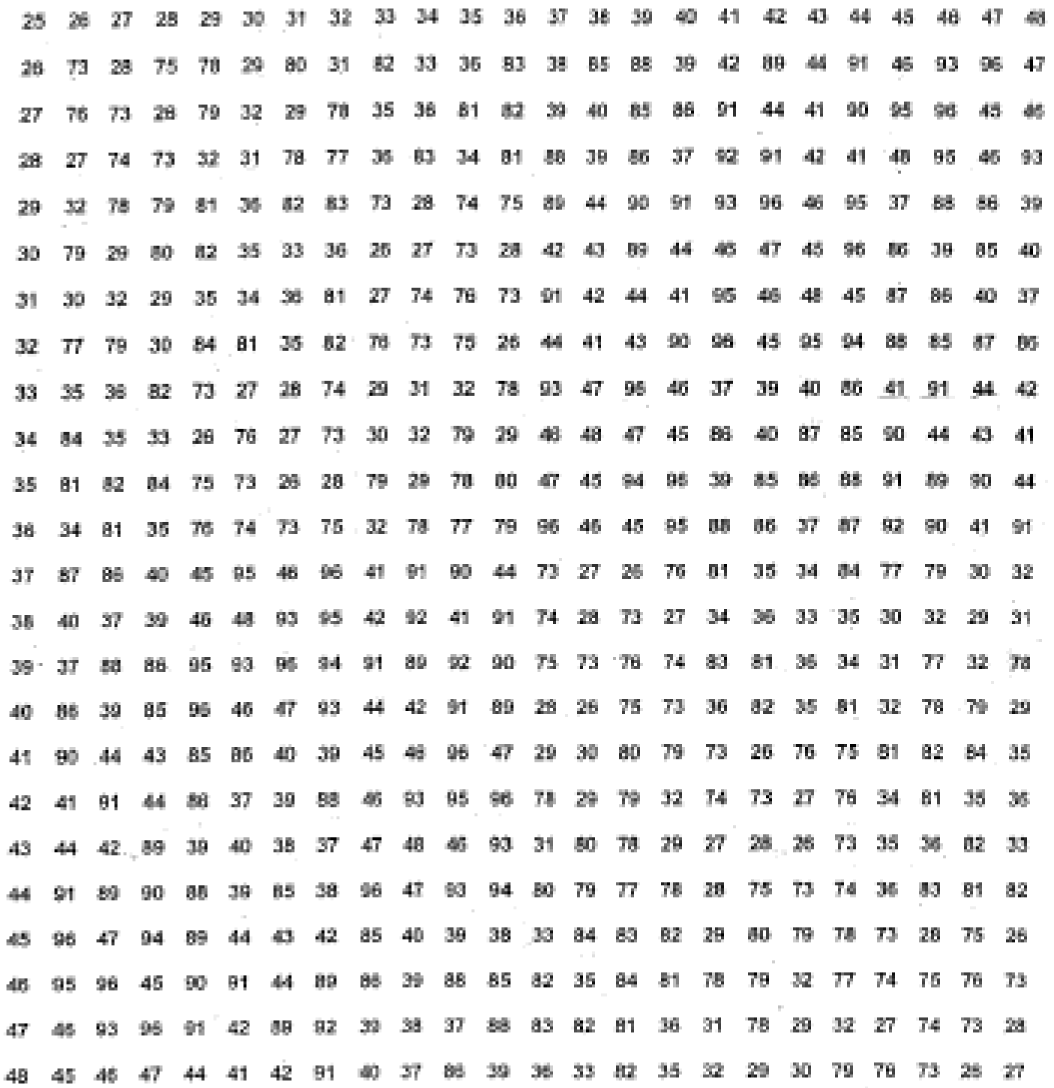
Table E.2: 1st component of the O_h^7 multiplication table



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
2	49	4	51	54	5	56	7	58	9	12	59	14	61	64	15	18	65	20	67	22	69	72	23
3	52	49	2	55	8	5	54	11	12	57	58	15	16	61	62	67	20	17	66	71	72	21	22
4	3	50	49	8	7	54	53	12	59	10	57	64	15	62	13	68	67	18	17	24	71	22	69
5	8	54	55	57	12	58	59	49	4	50	51	65	20	66	67	69	72	22	71	13	64	62	15
6	55	5	56	58	11	9	12	2	3	49	4	18	19	65	20	22	23	21	72	62	15	61	16
7	6	8	5	11	10	12	57	3	50	52	49	67	18	20	17	71	22	24	21	63	62	16	13
8	53	55	6	60	57	11	58	52	49	51	2	20	17	19	66	72	21	71	70	64	61	63	62
9	11	12	58	49	3	4	50	5	7	8	54	69	23	72	22	13	15	16	62	17	67	20	18
10	60	11	9	2	52	3	49	6	8	55	5	22	24	23	21	62	16	63	61	66	20	19	17
11	57	58	60	51	49	2	4	55	5	54	56	23	21	70	72	15	61	62	64	67	65	66	20
12	10	57	11	52	50	49	51	8	54	53	55	72	22	21	71	64	62	13	63	68	66	17	67
13	63	62	16	21	71	22	72	17	67	66	20	49	3	2	52	57	11	10	60	53	55	6	8
14	16	13	15	22	24	69	71	18	68	17	67	50	4	49	3	10	12	9	11	6	8	5	7
15	13	64	62	71	69	72	70	67	65	68	66	61	49	52	50	59	57	12	10	7	53	8	54
16	62	15	61	72	22	23	69	20	18	67	65	4	2	51	49	12	58	11	57	8	54	55	5
17	66	20	19	61	62	16	15	21	22	72	23	5	6	56	55	49	2	52	51	57	58	60	11
18	17	67	20	62	13	15	64	22	69	71	72	54	5	55	8	50	49	3	52	10	57	11	12
19	20	18	65	15	16	14	13	23	24	22	69	7	56	54	5	3	4	2	49	11	12	58	9
20	67	65	66	64	15	61	14	72	23	69	70	56	55	53	54	4	51	49	50	12	59	57	58
21	72	23	70	65	20	19	18	61	16	15	14	9	60	59	58	5	56	55	54	49	4	51	2
22	71	72	21	66	67	20	65	62	15	64	61	58	11	60	57	54	55	8	53	50	51	52	49
23	22	69	72	67	18	65	68	15	14	13	64	59	58	57	12	7	54	5	8	3	50	49	4
24	21	22	23	20	17	18	67	16	13	62	15	12	9	58	11	8	5	6	55	52	49	2	3

[1]

Table E.3: 2nd component of the O_h^7 multiplication table



25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
26	73	28	75	78	29	80	31	82	33	36	83	38	85	88	39	42	89	44	91	46	93	96	47
27	76	73	28	79	32	29	78	35	36	81	82	39	40	85	86	91	44	41	90	95	96	45	46
28	27	74	73	32	31	78	77	36	83	34	81	88	39	86	37	92	91	42	41	48	95	46	93
29	32	78	79	81	36	82	83	73	28	74	75	89	44	90	91	93	96	46	95	37	88	86	39
30	79	29	80	82	35	33	36	26	27	73	28	42	43	89	44	46	47	45	96	86	39	85	40
31	30	32	29	35	34	38	81	27	74	76	73	91	42	44	41	95	46	48	45	87	86	40	37
32	77	79	30	84	81	35	82	76	73	75	26	44	41	43	90	96	45	95	94	88	85	87	86
33	35	36	82	73	27	28	74	29	31	32	78	93	47	96	46	37	39	40	86	41	91	44	42
34	84	35	33	28	76	27	73	30	32	79	29	46	48	47	45	86	40	87	85	90	44	43	41
35	81	82	84	75	73	26	28	79	29	78	80	47	45	94	96	39	85	86	88	91	89	90	44
36	34	81	35	76	74	73	75	32	78	77	79	96	46	45	95	88	86	37	87	92	90	41	91
37	87	86	40	45	95	46	96	41	91	90	44	73	27	26	76	81	35	34	84	77	79	30	32
38	40	37	39	46	48	93	95	42	92	41	91	74	28	73	27	34	36	33	35	30	32	29	31
39	37	88	86	95	93	96	94	91	89	92	90	75	73	76	74	83	81	36	34	31	77	32	78
40	86	39	85	96	46	47	93	44	42	91	89	28	26	75	73	36	82	35	81	32	78	79	29
41	90	44	43	85	86	40	39	45	48	96	47	29	30	80	79	73	26	76	75	81	82	84	35
42	41	81	44	88	37	39	88	46	93	95	96	78	29	79	32	74	73	27	76	34	81	35	36
43	44	42	89	39	40	38	37	47	48	46	93	31	80	78	29	27	28	26	73	35	36	82	33
44	91	89	90	88	39	85	38	96	47	93	94	80	79	77	78	28	75	73	74	36	83	81	82
45	96	47	94	89	44	43	42	85	40	39	38	33	84	83	82	28	80	79	78	73	28	75	26
46	95	96	45	90	91	44	89	88	39	88	85	82	35	84	81	78	79	32	77	74	75	76	73
47	46	93	96	91	42	88	92	39	38	37	88	83	82	81	36	31	78	29	32	27	74	73	28
48	45	46	47	44	41	42	91	40	37	88	39	36	33	82	35	32	29	30	79	76	73	26	27

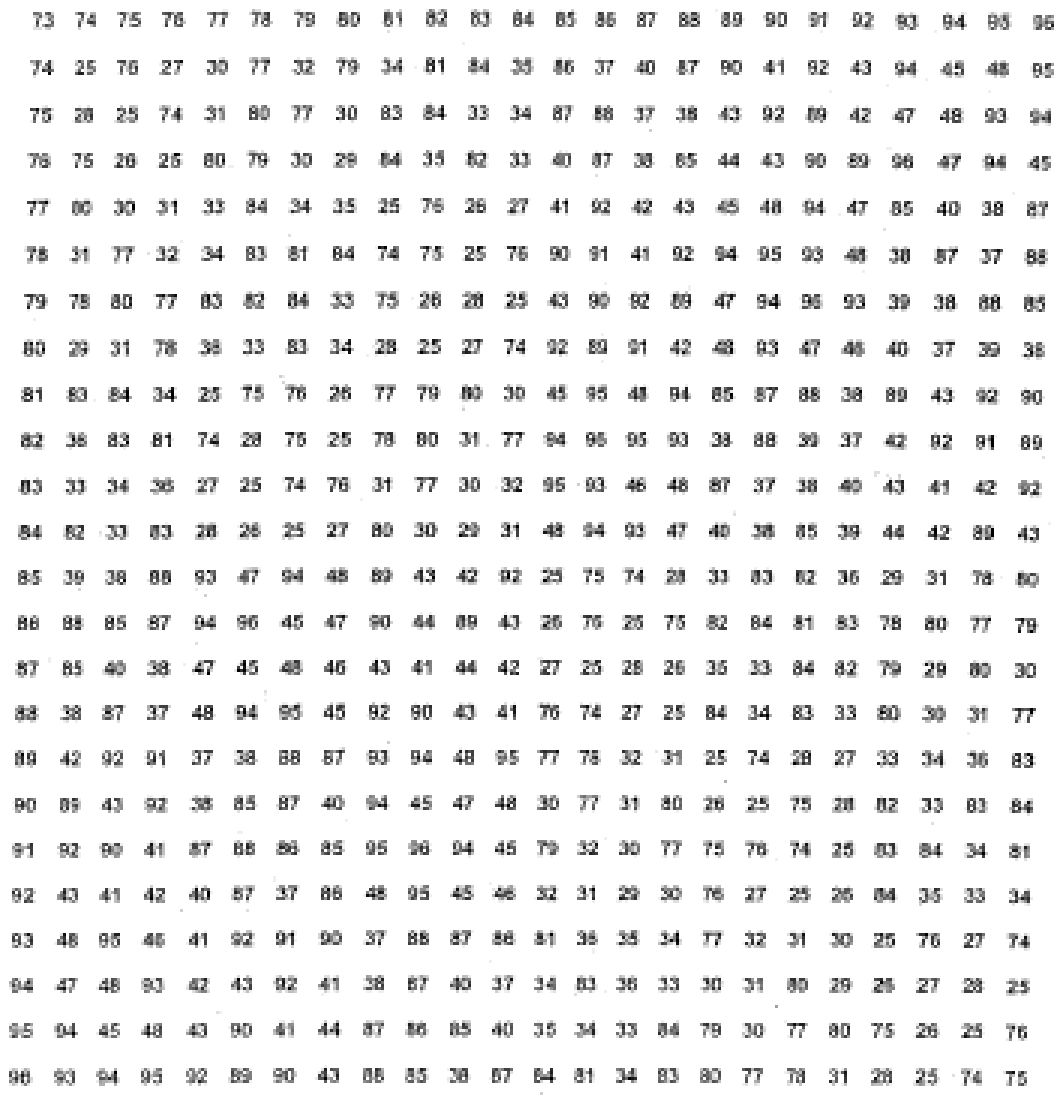
[2]

Table E.4: 3rd component of the O_h^7 multiplication table

49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72
50	1	52	3	6	53	8	55	10	57	60	11	62	13	16	63	66	17	6	19	70	21	24	71
51	4	1	50	7	56	53	6	59	60	9	10	63	64	13	14	19	68	65	18	23	24	69	70
52	51	2	1	56	55	6	5	60	11	58	9	16	63	14	61	20	19	66	65	72	23	70	21
53	56	6	7	9	60	10	11	1	52	2	3	17	68	18	19	21	24	70	23	61	16	14	63
54	7	53	8	10	59	57	60	50	51	1	52	66	67	17	68	70	71	69	24	14	63	13	64
55	54	56	53	59	58	60	9	51	2	4	1	19	66	68	65	23	70	72	69	15	14	64	61
56	5	7	54	12	9	59	10	4	1	3	50	68	65	67	18	24	69	23	22	16	13	15	14
57	59	60	10	1	51	52	2	53	55	56	6	21	71	24	70	61	63	64	14	65	19	68	66
58	12	59	57	50	4	61	1	54	56	7	53	70	72	71	69	14	64	15	13	18	68	67	65
59	9	10	12	3	1	50	52	7	53	5	6	71	69	22	24	63	13	14	16	19	17	18	66
60	58	9	59	4	2	1	3	56	6	5	7	24	70	69	23	16	14	61	15	20	18	65	19
61	15	14	64	69	23	70	24	65	19	18	68	1	51	50	4	9	59	58	12	5	7	54	56
62	64	61	63	70	72	21	23	66	20	65	19	2	62	1	51	58	60	57	59	54	56	53	55
63	61	16	14	23	21	24	22	19	17	20	18	3	1	4	2	11	9	60	58	55	5	56	6
64	14	63	13	24	70	71	21	68	66	19	17	52	50	3	1	60	10	59	9	56	6	7	53
65	18	68	67	13	14	64	63	69	70	24	71	53	54	8	7	1	50	4	3	9	10	12	59
66	65	19	68	14	61	63	16	70	21	23	24	6	53	7	56	2	1	51	4	58	9	59	60
67	68	66	17	63	64	62	61	71	72	70	21	55	8	6	53	51	52	56	1	59	60	10	57
68	19	17	18	16	63	13	62	24	71	21	22	8	7	5	6	52	3	1	2	60	11	9	10
69	24	71	22	17	68	67	66	13	64	63	62	57	12	11	10	53	8	7	6	1	52	3	50
70	23	24	69	18	19	68	17	14	63	16	13	10	59	12	9	6	7	56	5	2	3	4	1
71	70	21	24	19	66	17	20	63	62	61	16	11	10	9	60	55	6	53	56	51	2	1	52
72	69	70	71	68	65	66	19	64	61	14	63	60	57	10	59	56	53	54	7	4	1	50	51

[3]

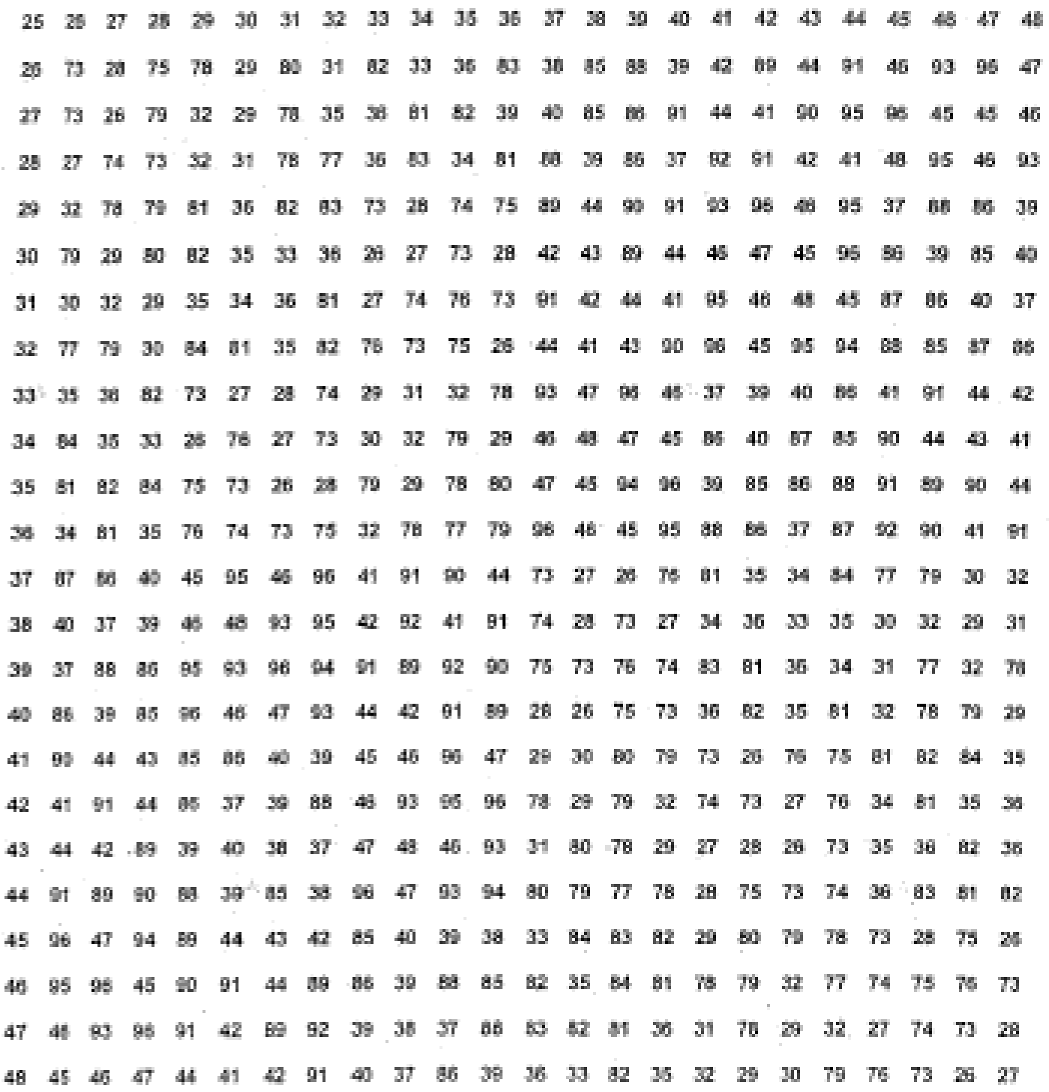
Table E.5: 4th component of the O_h^7 multiplication table



73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96
74	25	76	27	30	77	32	79	34	81	84	35	86	37	40	87	90	41	92	43	94	45	48	95
75	28	25	74	31	80	77	30	83	84	33	34	87	88	37	38	43	92	89	42	47	48	93	94
76	75	28	26	80	79	30	29	84	35	82	33	40	87	38	85	44	43	90	89	96	47	94	45
77	80	30	31	33	84	34	35	25	76	26	27	41	92	42	43	45	48	94	47	85	40	38	87
78	31	77	32	34	83	81	84	74	75	25	76	90	91	41	92	94	95	93	48	38	87	37	88
79	78	80	77	83	82	84	33	75	26	28	25	43	90	92	89	47	94	96	93	39	38	88	85
80	29	31	78	36	33	83	34	28	25	27	74	92	89	91	42	48	93	47	46	40	37	39	38
81	83	84	34	25	75	76	26	77	79	80	30	45	95	48	94	85	87	88	38	89	43	92	90
82	36	83	81	74	28	75	25	78	80	31	77	94	96	95	93	38	88	39	37	42	92	91	89
83	33	34	36	27	25	74	76	31	77	30	32	95	93	46	48	87	37	38	40	43	41	42	92
84	82	33	83	28	26	25	27	80	30	29	31	48	94	93	47	40	38	85	39	44	42	89	43
85	39	38	88	93	47	94	48	89	43	42	92	25	75	74	28	33	83	82	36	29	31	78	80
86	88	85	87	94	96	45	47	90	44	89	43	26	76	25	75	82	84	81	83	78	80	77	79
87	85	40	38	47	45	48	46	43	41	44	42	27	25	28	26	35	33	84	82	79	29	80	30
88	38	87	37	48	94	95	45	92	90	43	41	76	74	27	25	84	34	83	33	80	30	31	77
89	42	92	91	37	38	88	87	93	94	48	95	77	78	32	31	25	74	28	27	33	34	36	83
90	89	43	92	38	85	87	40	94	45	47	48	30	77	31	80	26	25	75	28	82	33	83	84
91	92	90	41	87	88	86	85	95	96	94	45	79	32	30	77	75	76	74	25	83	84	34	81
92	43	41	42	40	87	37	86	48	95	45	46	32	31	29	30	76	27	25	26	84	35	33	34
93	48	95	46	41	92	91	90	37	88	87	86	81	36	35	34	77	32	31	30	25	76	27	74
94	47	48	93	42	43	92	41	38	87	40	37	34	83	36	33	30	31	80	29	26	27	28	25
95	94	45	48	43	90	41	44	87	86	85	40	35	34	33	84	79	30	77	80	75	26	25	76
96	93	94	95	92	89	90	43	88	85	38	87	84	81	34	83	80	77	78	31	28	25	74	75

[4]

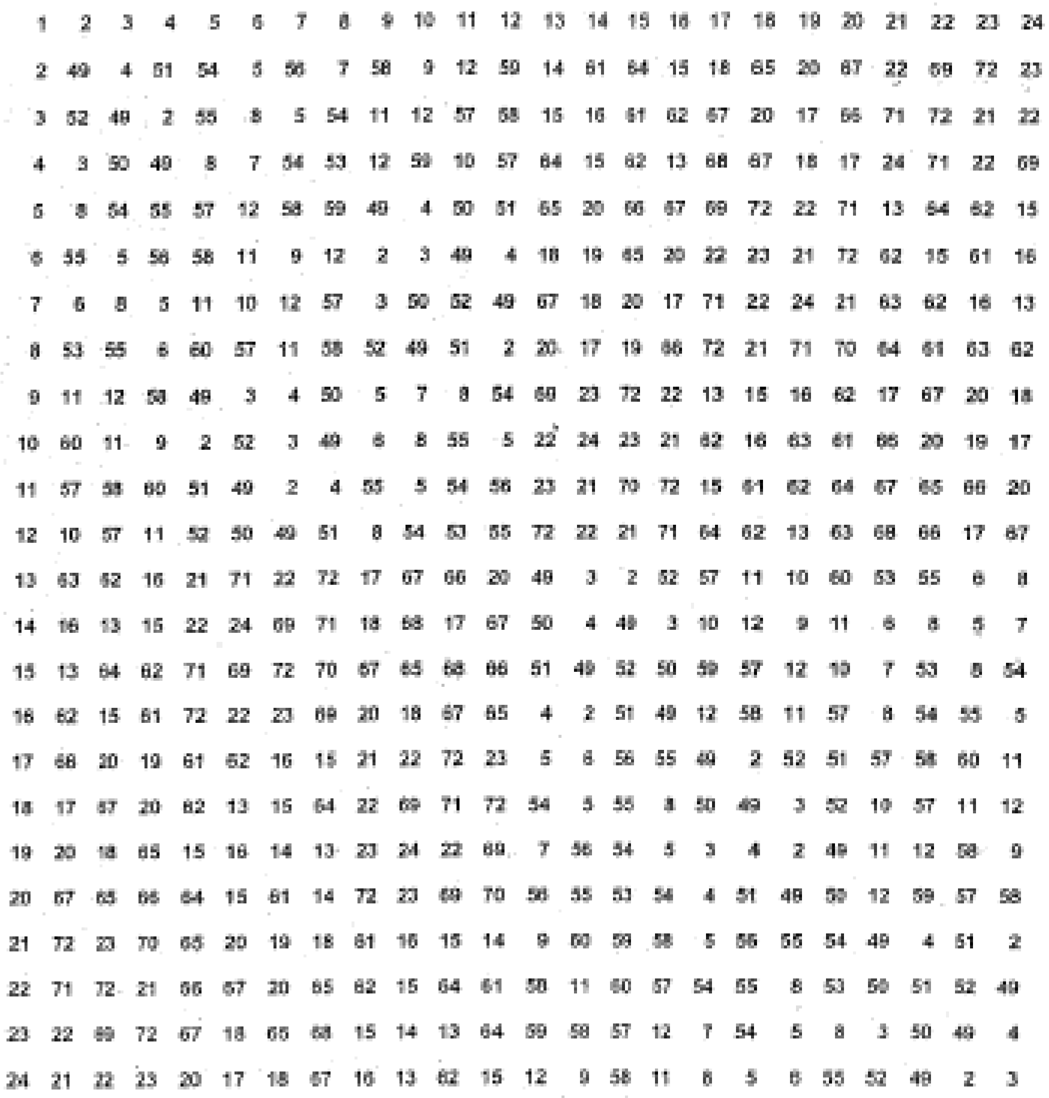
Table E.6: 5th component of the O_h^7 multiplication table



25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
26	73	28	75	78	29	80	31	82	33	36	83	38	85	88	39	42	89	44	91	46	93	96	47
27	73	26	79	32	29	78	35	38	81	82	39	40	85	86	91	44	41	90	95	96	45	45	46
28	27	74	73	32	31	78	77	36	83	34	81	88	39	86	37	92	91	42	41	48	95	46	93
29	32	78	79	81	36	82	83	73	28	74	75	89	44	90	91	93	96	48	95	37	88	86	39
30	79	29	80	82	35	33	36	26	27	73	28	42	43	89	44	46	47	45	96	86	39	85	40
31	30	32	29	35	34	36	81	27	74	76	73	91	42	44	41	95	46	48	45	87	86	40	37
32	77	79	30	84	81	35	82	76	73	75	26	44	41	43	90	96	45	95	94	88	85	87	86
33	35	38	82	73	27	28	74	29	31	32	78	93	47	96	46	37	39	40	86	41	91	44	42
34	84	35	33	26	76	27	73	30	32	79	29	46	48	47	45	86	40	87	85	90	44	43	41
35	81	82	84	75	73	26	28	79	29	78	80	47	45	94	96	39	85	86	88	91	89	90	44
36	34	81	35	76	74	73	75	32	78	77	79	96	46	45	95	88	86	37	87	92	90	41	91
37	87	86	40	45	95	46	96	41	91	90	44	73	27	26	76	81	35	34	84	77	79	30	32
38	40	37	39	46	48	93	95	42	92	41	91	74	28	73	27	34	36	33	35	30	32	29	31
39	37	88	86	95	93	96	94	91	89	92	90	75	73	76	74	83	81	36	34	31	77	32	78
40	86	39	85	96	46	47	93	44	42	91	89	28	26	75	73	36	82	35	81	32	78	79	29
41	90	44	43	85	86	40	39	45	46	96	47	29	30	80	79	73	26	76	75	81	82	84	35
42	41	91	44	86	37	39	88	46	93	95	96	78	29	79	32	74	73	27	76	34	81	35	36
43	44	42	89	39	40	38	37	47	48	46	93	31	80	78	29	27	28	26	73	35	36	82	36
44	91	89	90	88	39	85	38	96	47	93	94	80	79	77	78	28	75	73	74	36	83	81	82
45	96	47	94	89	44	43	42	85	40	39	38	33	84	83	82	29	80	79	78	73	28	75	26
46	95	96	45	90	91	44	89	86	39	88	85	82	35	84	81	78	79	32	77	74	75	76	73
47	48	93	96	91	42	89	92	39	38	37	88	83	82	81	36	31	78	29	32	27	74	73	28
48	45	46	47	44	41	42	91	40	37	86	39	36	33	82	35	32	29	30	79	76	73	26	27

[5]

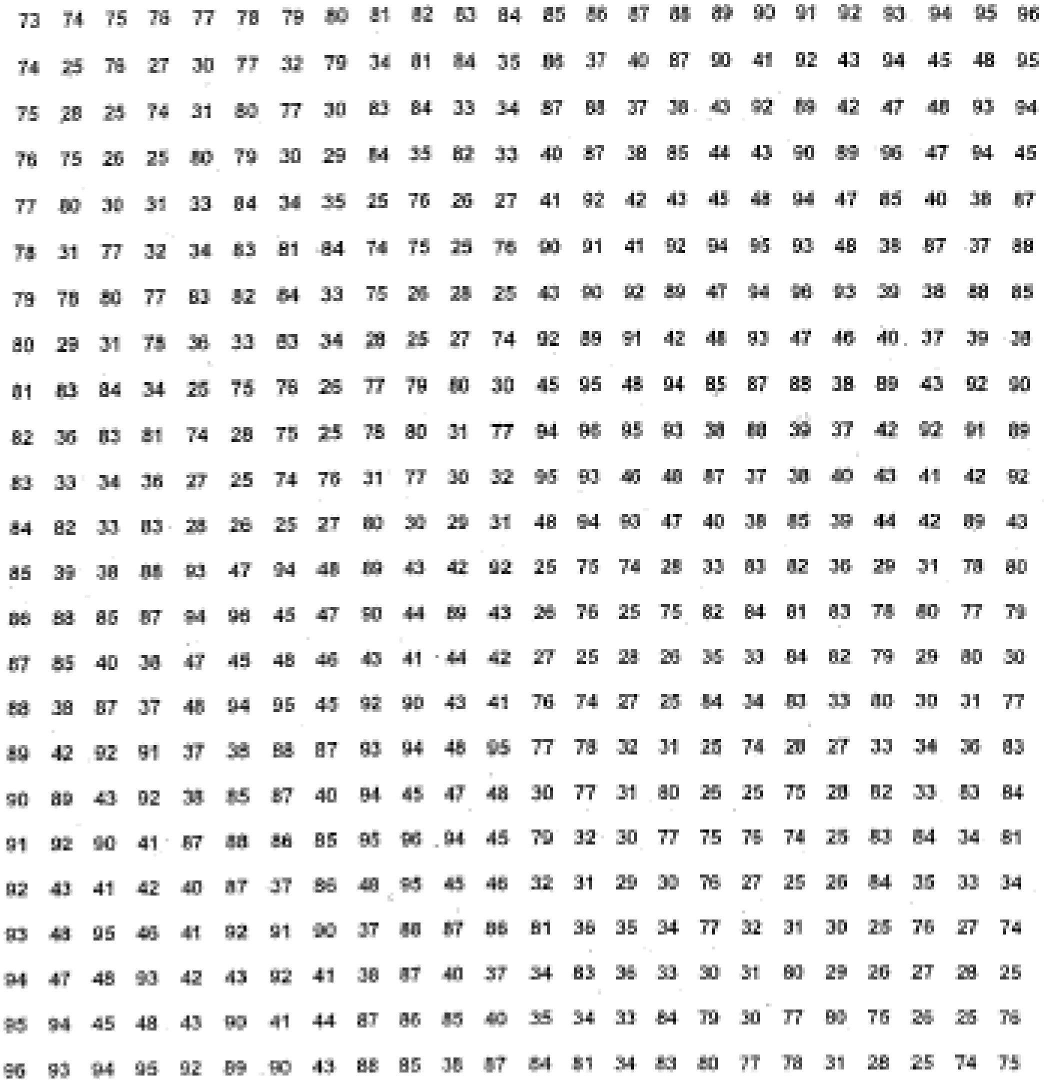
Table E.7: 6th component of the O_h^7 multiplication table



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
2	49	4	51	54	5	56	7	58	9	12	59	14	61	64	15	18	65	20	67	22	69	72	23
3	52	49	2	55	8	5	54	11	12	57	58	15	16	61	62	67	20	17	66	71	72	21	22
4	3	50	49	8	7	54	53	12	59	10	57	64	15	62	13	68	67	18	17	24	71	22	69
5	8	54	55	57	12	58	59	49	4	50	51	65	20	66	67	69	72	22	71	13	64	62	15
6	55	5	56	58	11	9	12	2	3	49	4	18	19	65	20	22	23	21	72	62	15	61	16
7	6	8	5	11	10	12	57	3	50	52	49	67	18	20	17	71	22	24	21	63	62	16	13
8	53	55	6	60	57	11	58	52	49	51	2	20	17	19	66	72	21	71	70	64	61	63	62
9	11	12	58	49	3	4	50	5	7	8	54	60	23	72	22	13	15	16	62	17	67	20	18
10	60	11	9	2	52	3	49	6	8	55	5	22	24	23	21	62	16	63	61	66	20	19	17
11	57	58	60	51	49	2	4	55	5	54	56	23	21	70	72	15	61	62	64	67	65	66	20
12	10	57	11	52	50	49	51	8	54	53	55	72	22	21	71	64	62	13	63	68	66	17	67
13	63	62	16	21	71	22	72	17	67	66	20	49	3	2	52	57	11	10	60	53	55	6	8
14	16	13	15	22	24	69	71	18	68	17	67	50	4	49	3	10	12	9	11	6	8	5	7
15	13	64	62	71	69	72	70	67	65	68	66	51	49	52	50	59	57	12	10	7	53	8	54
16	62	15	61	72	22	23	69	20	18	67	65	4	2	51	49	12	58	11	57	8	54	55	5
17	68	20	19	61	62	16	15	21	22	72	23	5	6	56	55	49	2	52	51	57	58	60	11
18	17	67	20	62	13	15	64	22	69	71	72	54	5	55	8	50	49	3	52	10	57	11	12
19	20	18	65	15	16	14	13	23	24	22	69	7	56	54	5	3	4	2	49	11	12	58	9
20	67	65	66	64	15	61	14	72	23	69	70	56	55	53	54	4	51	49	50	12	59	57	58
21	72	23	70	65	20	19	18	61	16	15	14	9	60	59	58	5	56	55	54	49	4	51	2
22	71	72	21	66	67	20	65	62	15	64	61	50	11	60	57	54	55	8	53	50	51	52	49
23	22	69	72	67	18	65	68	15	14	13	64	59	58	57	12	7	54	5	8	3	50	49	4
24	21	22	23	20	17	18	67	16	13	62	15	12	9	58	11	8	5	6	55	52	49	2	3

[6]

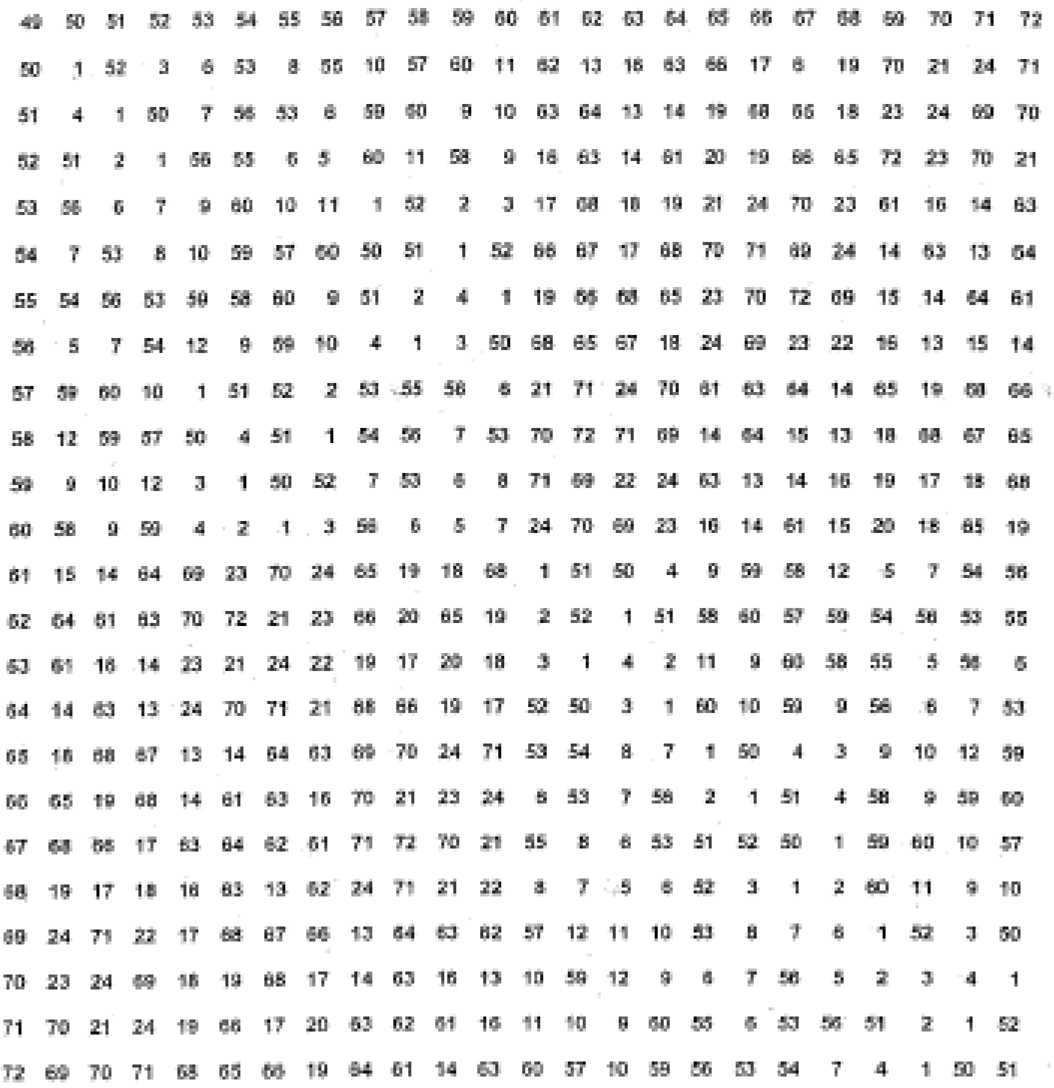
Table E.8: 7th component of the O_h^7 multiplication table



73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96
74	25	76	27	30	77	32	79	34	81	84	35	86	37	40	87	90	41	92	43	94	45	48	95
75	28	25	74	31	80	77	30	83	84	33	34	87	88	37	38	43	92	89	42	47	48	93	94
76	75	26	25	80	79	30	29	84	35	82	33	40	87	38	85	44	43	90	89	96	47	94	45
77	80	30	31	33	84	34	35	25	76	26	27	41	92	42	43	45	48	94	47	85	40	38	87
78	31	77	32	34	83	81	84	74	75	25	76	90	91	41	92	94	95	93	48	38	87	37	88
79	78	80	77	83	82	84	33	75	26	28	25	43	90	92	89	47	94	96	93	39	38	88	85
80	29	31	78	36	33	83	34	28	25	27	74	92	89	91	42	48	93	47	46	40	37	39	38
81	83	84	34	26	75	78	26	77	79	80	30	45	95	48	94	85	87	88	38	89	43	92	90
82	36	83	81	74	28	75	25	78	80	31	77	94	96	95	93	38	88	39	37	42	92	91	89
83	33	34	36	27	25	74	76	31	77	30	32	95	93	46	48	87	37	38	40	43	41	42	92
84	82	33	83	28	26	25	27	80	30	29	31	48	94	93	47	40	38	85	39	44	42	89	43
85	39	38	88	93	47	94	48	89	43	42	92	25	76	74	28	33	83	82	36	29	31	78	80
86	88	86	87	94	96	45	47	90	44	89	43	26	76	25	75	82	84	81	83	78	80	77	79
87	85	40	38	47	45	48	46	43	41	44	42	27	25	28	26	35	33	84	82	79	29	80	30
88	38	87	37	48	94	95	45	92	90	43	41	76	74	27	25	84	34	83	33	80	30	31	77
89	42	92	91	37	38	88	87	93	94	48	95	77	78	32	31	25	74	28	27	33	34	36	83
90	89	43	92	38	85	87	40	94	45	47	48	30	77	31	80	26	25	75	28	82	33	83	84
91	92	90	41	87	88	86	85	95	96	94	45	79	32	30	77	75	76	74	25	83	84	34	81
92	43	41	42	40	87	37	86	48	95	45	46	32	31	29	30	76	27	25	26	84	35	33	34
93	48	95	46	41	92	91	90	37	88	87	88	81	36	35	34	77	32	31	30	25	76	27	74
94	47	48	93	42	43	92	41	38	87	40	37	34	83	36	33	30	31	80	29	26	27	28	25
95	94	45	48	43	90	41	44	87	86	85	40	35	34	33	84	79	30	77	80	76	26	25	76
96	93	94	95	92	89	90	43	88	85	36	87	84	81	34	83	80	77	78	31	28	25	74	75

[7]

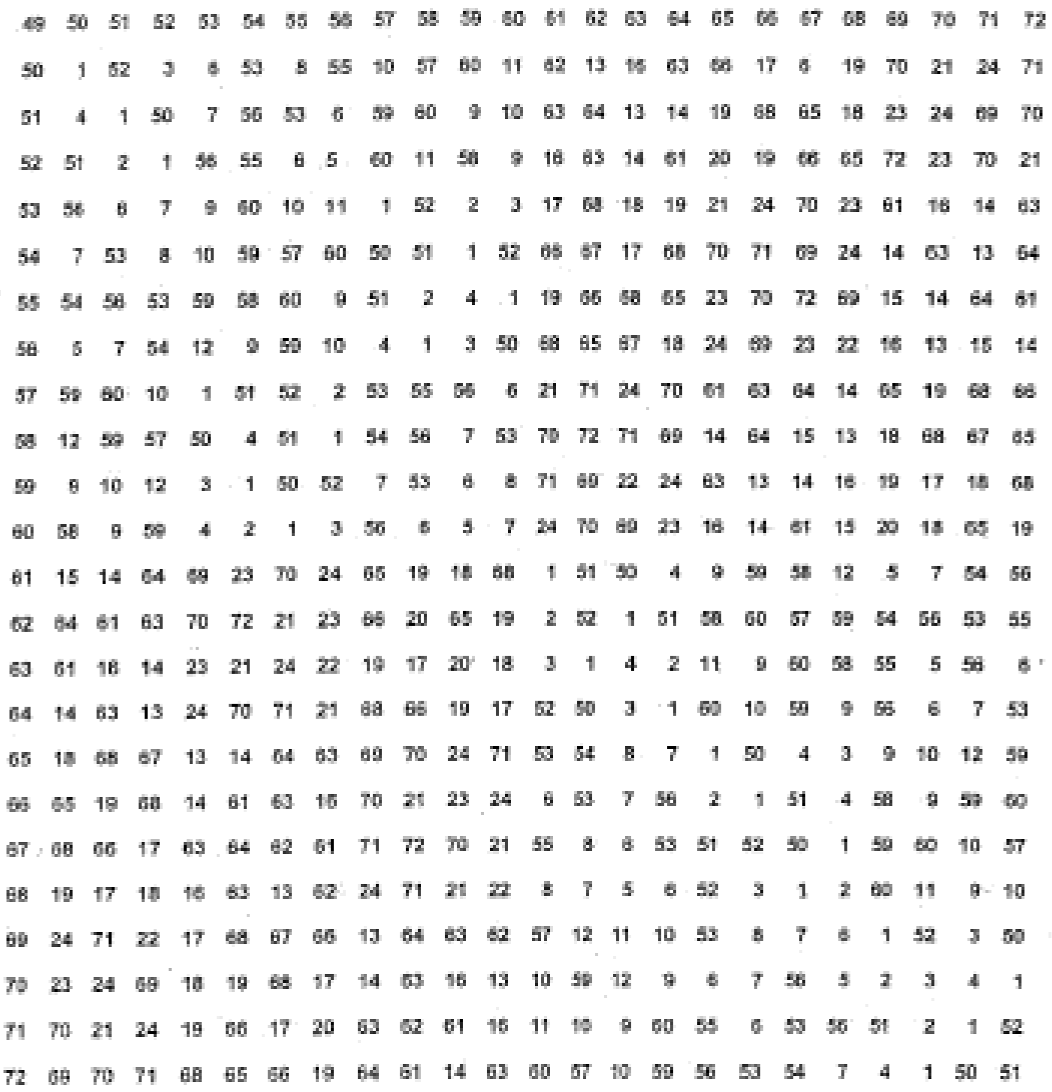
Table E.9: 8th component of the O_h^7 multiplication table



49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72
50	1	52	3	6	53	8	55	10	57	60	11	62	13	16	63	66	17	6	19	70	21	24	71
51	4	1	50	7	56	53	6	59	60	9	10	63	64	13	14	19	68	66	18	23	24	69	70
52	51	2	1	56	55	6	5	60	11	58	9	16	63	14	61	20	19	66	65	72	23	70	21
53	56	6	7	9	60	10	11	1	52	2	3	17	68	18	19	21	24	70	23	61	16	14	63
54	7	53	8	10	59	57	60	50	51	1	52	66	67	17	68	70	71	69	24	14	63	13	64
55	54	56	53	59	58	60	9	51	2	4	1	19	66	68	65	23	70	72	69	15	14	64	61
56	5	7	54	12	9	59	10	4	1	3	50	68	65	67	18	24	69	23	22	16	13	15	14
57	59	60	10	1	51	52	2	53	55	56	6	21	71	24	70	61	63	64	14	65	19	68	66
58	12	59	57	50	4	51	1	54	56	7	53	70	72	71	69	14	64	15	13	18	68	67	65
59	9	10	12	3	1	50	52	7	53	6	8	71	69	22	24	63	13	14	16	19	17	18	68
60	58	9	59	4	2	1	3	56	6	5	7	24	70	69	23	16	14	61	15	20	18	65	19
61	15	14	64	69	23	70	24	65	19	18	68	1	51	50	4	9	59	58	12	5	7	54	56
62	64	61	63	70	72	21	23	66	20	65	19	2	52	1	51	58	60	57	59	54	56	53	55
63	61	16	14	23	21	24	22	19	17	20	18	3	1	4	2	11	9	60	58	55	5	56	6
64	14	63	13	24	70	71	21	68	66	19	17	52	50	3	1	60	10	59	9	56	6	7	53
65	16	68	67	13	14	64	63	69	70	24	71	53	54	8	7	1	50	4	3	9	10	12	59
66	65	19	68	14	61	63	16	70	21	23	24	6	53	7	56	2	1	51	4	58	9	59	60
67	68	66	17	63	64	62	61	71	72	70	21	55	8	6	53	51	52	50	1	59	60	10	57
68	19	17	18	16	63	13	62	24	71	21	22	8	7	5	6	52	3	1	2	60	11	9	10
69	24	71	22	17	68	67	66	13	64	63	62	57	12	11	10	53	8	7	6	1	52	3	50
70	23	24	69	18	19	68	17	14	63	16	13	10	59	12	9	6	7	56	5	2	3	4	1
71	70	21	24	19	66	17	20	63	62	61	16	11	10	9	60	55	6	53	56	51	2	1	52
72	69	70	71	68	65	66	19	64	61	14	63	60	57	10	59	56	53	54	7	4	1	50	51

[8]

Table E.10: 9th component of the O_h^7 multiplication table



49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72
50	1	52	3	6	53	8	55	10	57	60	11	62	13	16	63	66	17	6	19	70	21	24	71
51	4	1	50	7	56	53	6	59	60	9	10	63	64	13	14	19	68	65	18	23	24	69	70
52	51	2	1	56	55	6	5	60	11	58	9	16	63	14	61	20	19	66	65	72	23	70	21
53	56	6	7	9	60	10	11	1	52	2	3	17	68	18	19	21	24	70	23	61	16	14	63
54	7	53	8	10	59	57	60	50	51	1	52	69	67	17	68	70	71	69	24	14	63	13	64
55	54	58	53	59	58	60	9	51	2	4	1	19	66	68	65	23	70	72	69	15	14	64	61
56	5	7	54	12	9	59	10	4	1	3	50	68	65	67	18	24	69	23	22	16	13	15	14
57	59	60	10	1	61	52	2	53	55	56	6	21	71	24	70	61	63	64	14	65	19	68	66
58	12	59	57	50	4	61	1	54	56	7	53	70	72	71	69	14	64	15	13	18	68	67	65
59	8	10	12	3	1	50	52	7	53	6	8	71	69	22	24	63	13	14	16	19	17	18	68
60	58	9	59	4	2	1	3	56	6	5	7	24	70	69	23	16	14	61	15	20	18	65	19
61	15	14	64	69	23	70	24	65	19	18	68	1	51	50	4	9	59	58	12	5	7	54	56
62	64	61	63	70	72	21	23	66	20	65	19	2	52	1	51	58	60	57	59	54	56	53	55
63	61	16	14	23	21	24	22	19	17	20	18	3	1	4	2	11	9	60	58	55	5	56	6
64	14	63	13	24	70	71	21	68	66	19	17	52	50	3	1	60	10	59	9	56	6	7	53
65	18	68	67	13	14	64	63	69	70	24	71	53	54	8	7	1	50	4	3	9	10	12	59
66	65	19	68	14	61	63	16	70	21	23	24	6	53	7	56	2	1	51	4	58	9	59	60
67	68	66	17	63	64	62	61	71	72	70	21	55	8	6	53	51	52	50	1	59	60	10	57
68	19	17	18	16	63	13	62	24	71	21	22	8	7	5	6	52	3	1	2	60	11	9	10
69	24	71	22	17	68	67	66	13	64	63	62	57	12	11	10	53	8	7	6	1	52	3	60
70	23	24	69	18	19	68	17	14	63	16	13	10	59	12	9	6	7	56	5	2	3	4	1
71	70	21	24	19	66	17	20	63	62	61	16	11	16	9	60	55	6	53	56	51	2	1	52
72	69	70	71	68	65	66	19	64	61	14	63	60	57	10	59	56	53	54	7	4	1	50	51

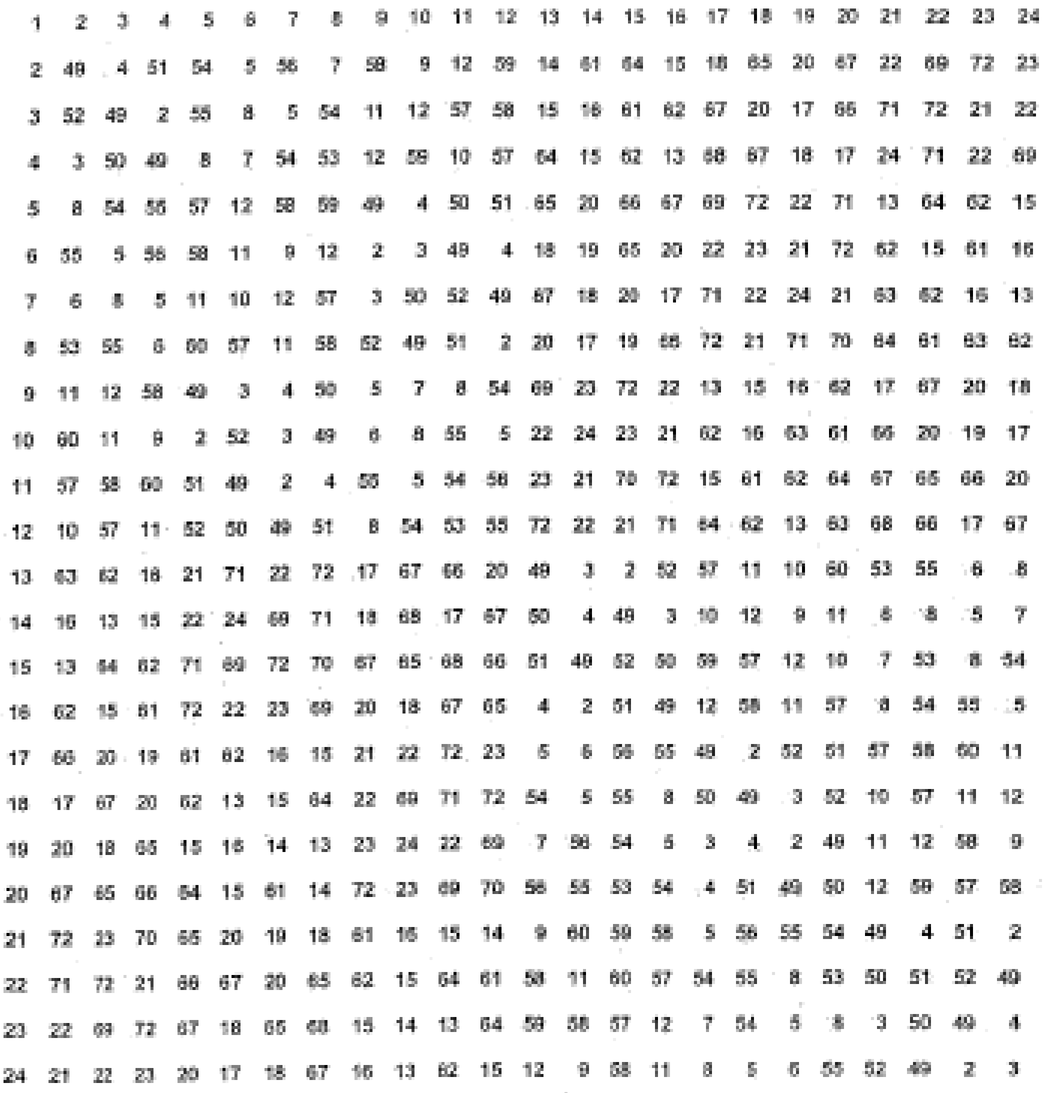
[9]

Table E.11: 10th component of the O_h^7 multiplication table

73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96
74	25	76	27	30	77	32	79	34	81	84	35	86	37	40	87	90	41	92	43	94	45	48	95
75	28	25	74	31	80	77	30	83	84	33	34	87	88	37	38	43	92	89	42	47	48	93	94
76	75	26	25	80	79	30	29	84	35	82	33	40	87	38	85	44	43	90	89	96	47	94	45
77	80	30	31	33	84	34	35	26	76	26	27	41	92	42	43	45	48	94	47	85	40	38	87
78	31	77	32	34	83	81	84	74	75	25	76	90	91	41	92	94	95	93	48	38	87	37	88
79	78	80	77	83	82	84	33	75	26	28	25	43	90	92	89	47	94	96	93	39	38	88	85
80	29	31	78	38	33	83	34	28	25	27	74	92	89	91	42	48	93	47	46	40	37	39	38
81	83	84	34	25	75	76	26	77	79	80	30	45	95	48	94	85	87	88	38	89	43	92	90
82	36	83	81	74	28	75	25	78	80	31	77	94	96	95	93	38	88	39	37	42	92	91	89
83	33	34	36	27	25	74	76	31	77	30	32	95	93	46	48	87	37	38	40	43	41	42	92
84	82	33	83	28	26	25	27	80	30	29	31	48	84	93	47	40	38	85	39	44	42	89	43
85	39	38	88	93	47	94	48	89	43	42	92	25	75	74	28	33	83	82	36	29	31	78	80
86	88	85	87	94	96	45	47	90	44	89	43	26	76	25	75	82	84	81	83	78	80	77	79
87	85	40	38	47	45	48	46	43	41	44	42	27	25	28	26	35	33	84	82	79	29	80	30
88	38	87	37	48	94	96	45	92	90	43	41	76	74	27	25	84	34	83	33	80	30	31	77
89	42	92	91	37	38	88	87	93	94	48	95	77	78	32	31	25	74	28	27	33	34	36	83
90	89	43	92	38	86	87	40	94	45	47	48	30	77	31	80	28	25	75	28	82	33	83	84
91	92	90	41	87	88	86	85	95	96	94	45	79	32	30	77	75	76	74	25	83	84	34	81
92	43	41	42	40	87	37	86	48	95	45	46	32	31	29	30	76	27	25	26	84	35	33	34
93	48	95	46	41	92	91	90	37	88	87	86	81	36	35	34	77	32	31	30	25	76	27	74
94	47	48	93	42	43	92	41	38	87	40	37	34	83	36	33	30	31	80	29	26	27	28	25
95	94	46	48	43	90	41	44	87	86	85	40	35	34	33	84	79	30	77	80	75	26	25	76
96	93	94	95	92	89	90	43	88	86	38	87	84	81	34	83	80	77	78	31	28	25	74	75

[10]

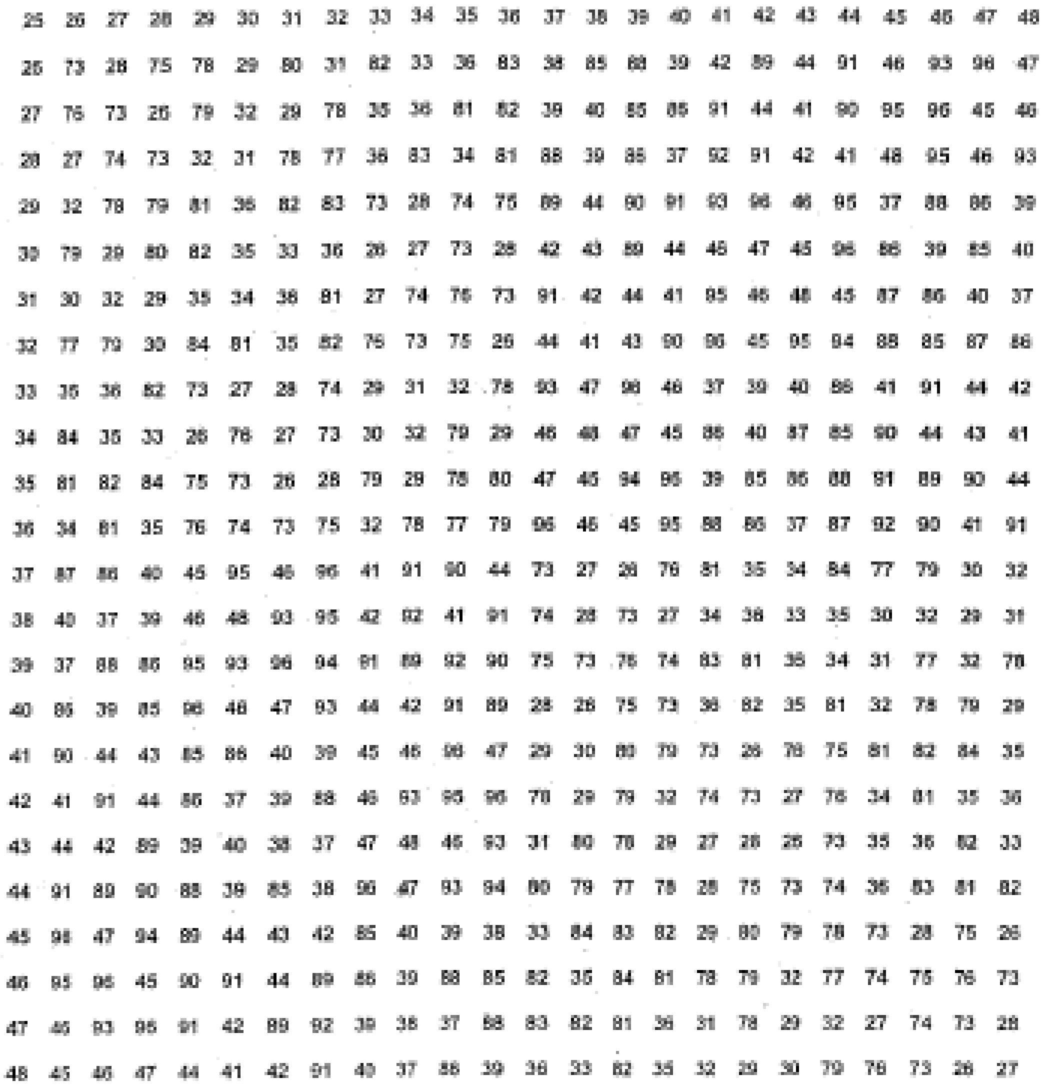
Table E.12: 11th component of the O_h^7 multiplication table



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
2	49	4	51	54	5	56	7	58	9	12	59	14	61	64	15	18	65	20	67	22	69	72	23
3	52	49	2	55	8	5	54	11	12	57	58	15	16	61	62	67	20	17	66	71	72	21	22
4	3	50	49	8	7	54	53	12	59	10	57	64	15	62	13	68	67	18	17	24	71	22	69
5	8	54	56	57	12	58	59	49	4	50	51	65	20	66	67	69	72	22	71	13	64	62	15
6	55	5	56	58	11	9	12	2	3	49	4	18	19	65	20	22	23	21	72	62	15	61	16
7	6	8	5	11	10	12	57	3	50	52	49	67	18	20	17	71	22	24	21	63	62	16	13
8	53	55	6	60	57	11	58	62	49	51	2	20	17	19	66	72	21	71	70	64	61	63	62
9	11	12	58	49	3	4	50	5	7	8	54	69	23	72	22	13	15	16	62	17	67	20	18
10	60	11	9	2	52	3	49	6	8	55	5	22	24	23	21	62	16	63	61	66	20	19	17
11	57	58	60	51	49	2	4	56	5	54	58	23	21	70	72	15	61	62	64	67	65	66	20
12	10	57	11	52	50	49	51	8	54	53	55	72	22	21	71	64	62	13	63	68	66	17	67
13	63	62	16	21	71	22	72	17	67	66	20	49	3	2	52	57	11	10	60	53	55	6	8
14	16	13	15	22	24	69	71	18	68	17	67	50	4	49	3	10	12	9	11	6	8	5	7
15	13	64	62	71	69	72	70	67	65	68	66	51	49	52	50	59	57	12	10	7	53	8	54
16	62	15	61	72	22	23	69	20	18	67	65	4	2	51	49	12	58	11	57	8	54	55	5
17	66	20	19	61	62	16	15	21	22	72	23	5	6	56	55	49	2	52	51	57	58	60	11
18	17	67	20	62	13	15	64	22	69	71	72	54	5	55	8	50	49	3	52	10	57	11	12
19	20	18	65	15	16	14	13	23	24	22	69	7	56	54	5	3	4	2	49	11	12	58	9
20	67	65	66	64	15	61	14	72	23	69	70	56	55	53	54	4	51	49	50	12	59	57	58
21	72	23	70	66	20	19	18	61	16	15	14	9	60	59	58	5	56	55	54	49	4	51	2
22	71	72	21	66	67	20	65	62	15	64	61	58	11	60	57	54	55	8	53	50	51	52	49
23	22	69	72	67	18	66	68	15	14	13	64	59	58	57	12	7	54	5	8	3	50	49	4
24	21	22	23	20	17	18	67	16	13	62	15	12	9	68	11	8	5	6	55	52	49	2	3

[11]

Table E.13: 12th component of the O_h^7 multiplication table



25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
26	73	28	75	78	29	80	31	82	33	36	83	38	85	88	39	42	89	44	91	46	93	96	47
27	76	73	26	79	32	29	78	35	36	81	82	39	40	85	86	91	44	41	90	95	96	45	46
28	27	74	73	32	31	78	77	36	83	34	81	88	39	86	37	92	91	42	41	48	95	46	93
29	32	78	79	81	36	82	83	73	28	74	75	89	44	90	91	93	96	46	95	37	88	86	39
30	79	29	80	82	35	33	36	26	27	73	28	42	43	89	44	46	47	45	96	86	39	85	40
31	30	32	29	35	34	38	81	27	74	76	73	91	42	44	41	85	46	48	45	87	86	40	37
32	77	79	30	84	81	35	82	76	73	75	26	44	41	43	90	96	45	95	94	88	85	87	86
33	35	36	82	73	27	28	74	29	31	32	78	93	47	96	46	37	39	40	86	41	91	44	42
34	84	35	33	26	78	27	73	30	32	79	29	46	48	47	45	86	40	87	85	90	44	43	41
35	81	82	84	75	73	26	28	79	29	78	80	47	45	94	96	39	85	86	88	91	89	90	44
36	34	81	35	76	74	73	75	32	78	77	79	96	46	45	95	88	86	37	87	92	90	41	91
37	87	86	40	45	95	46	96	41	91	90	44	73	27	28	76	81	35	34	84	77	79	30	32
38	40	37	39	46	48	93	95	42	92	41	91	74	28	73	27	34	36	33	35	30	32	29	31
39	37	88	86	95	93	96	94	91	89	92	90	75	73	76	74	83	81	36	34	31	77	32	78
40	86	39	85	96	48	47	93	44	42	91	89	28	26	75	73	36	82	35	81	32	78	79	29
41	90	44	43	85	88	40	39	45	46	96	47	29	30	80	79	73	26	78	75	81	82	84	35
42	41	91	44	86	37	39	88	46	93	95	96	78	29	79	32	74	73	27	76	34	81	35	36
43	44	42	89	39	40	38	37	47	48	45	93	31	80	78	29	27	28	26	73	35	36	82	33
44	91	89	90	88	39	85	38	96	47	93	94	80	79	77	78	28	75	73	74	36	83	81	82
45	96	47	94	89	44	43	42	85	40	39	38	33	84	83	82	29	80	79	78	73	28	75	26
46	95	96	45	90	91	44	89	86	39	88	85	82	35	84	81	78	79	32	77	74	75	76	73
47	46	93	96	91	42	89	92	39	38	37	88	83	82	81	36	31	78	29	32	27	74	73	28
48	45	46	47	44	41	42	91	40	37	88	39	36	33	82	35	32	29	30	79	76	73	26	27

[12]

Table E.14: 13th component of the O_h^7 multiplication table

73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96
74	25	76	27	30	77	32	79	34	81	84	35	86	37	40	87	90	41	92	43	94	45	48	95
75	28	25	74	31	80	77	30	83	84	33	34	87	88	37	38	43	92	89	42	47	48	93	94
76	75	26	25	80	79	30	29	84	35	82	33	40	87	38	85	44	43	90	89	96	47	94	45
77	80	30	31	33	84	34	35	25	76	26	27	41	92	42	43	45	48	94	47	85	40	38	87
78	31	77	32	34	83	81	84	74	75	25	76	90	91	41	92	94	95	93	48	38	87	37	88
79	78	80	77	83	82	84	33	75	26	28	25	43	90	92	89	47	94	96	93	39	38	88	85
80	29	31	78	36	33	83	34	28	25	27	74	92	89	91	42	48	93	47	46	40	37	39	38
81	83	84	34	25	75	76	26	77	79	80	30	45	95	48	94	85	87	88	38	89	43	92	90
82	36	83	81	74	28	75	25	78	80	31	77	94	96	95	93	38	88	39	37	42	92	91	89
83	33	34	36	27	25	74	76	31	77	30	32	95	93	46	48	87	37	38	40	43	41	42	92
84	82	33	83	28	26	25	27	80	30	29	31	48	94	93	47	46	38	85	39	44	42	89	43
85	39	38	88	93	47	94	48	89	43	42	92	25	75	74	28	33	83	82	36	29	31	78	80
86	88	85	87	94	96	45	47	90	44	89	43	26	76	25	75	82	84	81	83	78	80	77	79
87	85	40	38	47	45	48	46	43	41	44	42	27	25	28	26	35	33	84	82	79	29	80	30
88	38	87	37	48	94	96	45	92	90	43	41	76	74	27	25	84	34	83	33	80	30	31	77
89	42	92	91	37	38	88	87	93	94	48	95	77	78	32	31	25	74	28	27	33	34	36	83
90	89	43	92	38	85	87	40	94	45	47	48	30	77	31	80	26	25	75	28	82	33	83	84
91	92	90	41	87	88	86	85	95	96	94	45	79	32	30	77	75	76	74	25	83	84	34	81
92	43	41	42	40	87	37	86	48	95	45	46	32	31	29	30	76	27	25	26	84	35	33	34
93	48	95	46	41	92	91	90	37	88	87	86	81	36	35	34	77	32	31	30	25	76	27	74
94	47	48	83	42	43	92	41	38	87	40	37	34	83	36	33	30	31	80	29	26	27	28	25
95	94	45	48	43	90	41	44	87	86	85	40	35	34	33	84	79	30	77	80	75	26	25	76
96	93	94	95	92	89	90	43	88	85	38	87	84	81	34	83	80	77	78	31	28	25	74	75

[13]

Table E.15: 14th component of the O_h^7 multiplication table

49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72
50	1	52	3	6	53	8	55	10	57	60	11	62	13	16	63	66	17	6	19	70	21	24	71
51	4	1	50	7	56	53	6	59	60	9	10	63	64	13	14	19	66	65	18	23	24	69	70
52	51	2	1	56	55	6	5	60	11	58	9	16	63	14	61	20	19	66	65	72	23	70	21
53	56	6	7	9	60	10	11	1	52	2	3	17	68	18	19	21	24	70	23	61	16	14	63
54	7	53	8	10	58	57	60	50	51	1	52	66	67	17	68	70	71	69	24	14	63	13	64
55	54	56	53	59	58	60	9	51	2	4	1	19	66	68	65	23	70	72	69	15	14	64	61
56	5	7	54	12	9	59	10	4	1	3	50	68	65	67	18	24	69	23	22	16	13	15	14
57	59	60	10	1	51	52	2	53	55	56	6	21	71	24	70	61	63	64	14	65	19	68	66
58	12	59	57	50	4	51	1	54	56	7	53	70	72	71	69	14	64	15	13	18	68	67	65
59	9	10	12	3	1	50	52	7	53	6	8	71	69	22	24	63	13	14	16	19	17	18	68
60	58	9	59	4	2	1	3	56	6	5	7	24	70	69	23	16	14	61	15	20	18	65	19
61	15	14	64	69	23	70	24	65	19	18	68	1	51	50	4	9	59	58	12	5	7	54	56
62	64	61	63	70	72	21	23	66	20	65	19	2	52	1	51	58	60	57	59	54	56	53	55
63	61	16	14	23	21	24	22	19	17	20	18	3	1	4	2	11	9	60	58	55	5	56	6
64	14	63	13	24	70	71	21	68	66	19	17	52	50	3	1	60	10	59	9	56	6	7	53
65	18	68	67	13	14	64	63	69	70	24	71	53	54	8	7	1	50	4	3	9	10	12	59
66	65	19	68	14	61	63	16	70	21	23	24	6	53	7	56	2	1	51	4	58	9	59	60
67	68	66	17	63	64	62	61	71	72	70	21	55	8	6	53	51	52	50	1	59	60	10	57
68	19	17	18	16	63	13	62	24	71	21	22	8	7	5	6	52	3	1	2	60	11	9	10
69	24	71	22	17	68	67	66	13	64	63	62	57	12	11	10	53	8	7	6	1	52	3	50
70	23	24	69	18	19	68	17	14	63	16	13	10	59	12	9	6	7	58	5	2	3	4	1
71	70	21	24	19	66	17	20	63	62	61	16	11	10	9	60	55	6	53	56	51	2	1	52
72	69	70	71	68	65	66	19	64	61	14	63	60	57	10	59	56	53	54	7	4	1	50	51

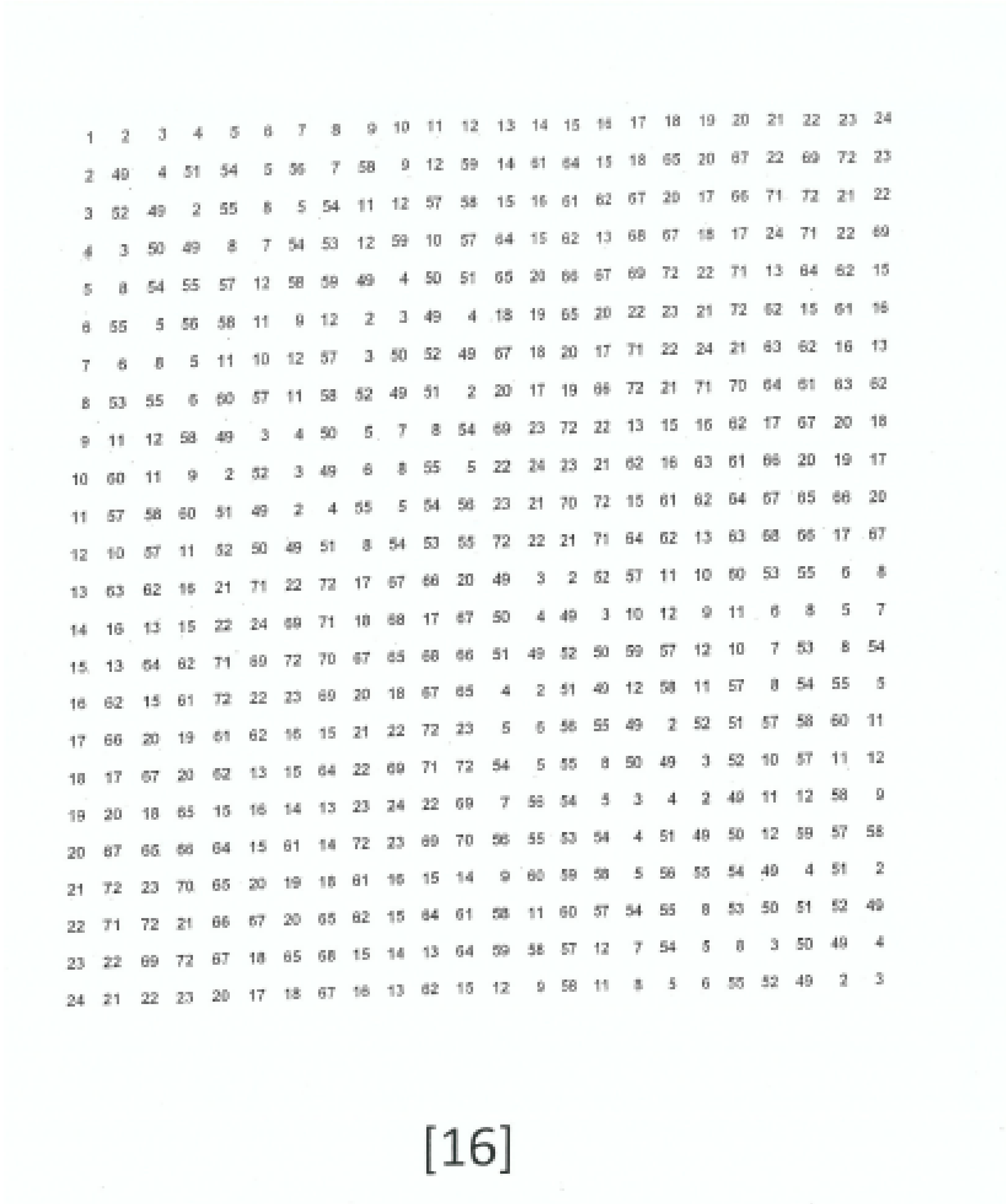
[14]

Table E.16: 15th component of the O_h^7 multiplication table

25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
26	73	28	75	76	29	80	31	82	33	36	83	38	85	88	39	42	89	44	91	46	93	96	47
27	76	73	26	79	32	29	78	35	36	81	82	39	40	85	86	91	44	41	90	95	96	45	46
28	27	74	73	32	31	78	77	36	83	34	81	88	39	86	37	92	91	42	41	48	95	46	93
29	32	78	79	81	36	82	83	73	28	74	75	89	44	90	91	93	96	46	95	37	88	86	39
30	79	29	80	82	35	33	36	26	27	73	28	42	43	89	44	46	47	45	96	88	39	85	40
31	30	32	29	35	34	36	81	27	74	76	73	91	42	44	41	95	46	48	45	87	86	40	37
32	77	79	30	84	81	35	82	76	73	75	26	44	41	43	90	96	45	95	94	88	85	87	86
33	35	36	82	73	27	28	74	29	31	32	78	93	47	96	46	37	39	40	86	41	91	44	42
34	84	35	33	26	76	27	73	30	32	79	29	46	48	47	45	86	40	87	85	90	44	43	41
35	81	82	84	75	73	26	28	79	29	76	80	47	45	94	96	39	85	86	88	91	89	90	44
36	34	81	35	76	74	73	75	32	78	77	79	96	46	45	95	88	86	37	87	92	90	41	91
37	87	88	40	45	95	46	96	41	91	90	44	73	27	28	76	81	35	34	84	77	79	30	32
38	40	37	39	46	48	93	95	42	92	41	91	74	28	73	27	34	36	33	35	30	32	29	31
39	37	88	86	95	93	96	94	91	89	92	90	75	73	76	74	83	81	36	34	31	77	32	78
40	86	39	85	96	46	47	93	44	42	91	89	28	26	75	73	36	82	35	81	32	78	79	29
41	90	44	43	85	86	40	39	45	46	96	47	29	30	80	79	73	26	76	75	81	82	84	35
42	41	91	44	86	37	39	88	46	93	95	96	78	29	79	32	74	73	27	76	34	81	35	36
43	44	42	89	39	40	38	37	47	48	46	93	31	80	78	29	27	28	26	73	35	36	82	33
44	91	89	90	88	39	85	38	96	47	93	94	80	79	77	78	28	75	73	74	36	83	81	82
45	96	47	94	89	44	43	42	85	40	39	38	33	84	83	82	29	80	79	78	73	28	75	26
46	95	96	45	90	91	44	89	86	39	88	85	82	35	84	81	78	79	32	77	74	75	76	73
47	46	93	96	91	42	89	92	39	38	37	88	83	82	81	35	31	78	29	32	27	74	73	28
48	45	46	47	44	41	42	91	40	37	86	39	36	33	82	35	32	29	30	79	76	73	26	27

[15]

Table E.17: 16th component of the O_h^7 multiplication table



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
2	49	4	51	54	5	56	7	58	9	12	59	14	61	64	15	18	65	20	67	22	69	72	23
3	52	49	2	55	8	5	54	11	12	57	58	15	16	61	62	67	20	17	66	71	72	21	22
4	3	50	49	8	7	54	53	12	59	10	57	64	15	62	13	68	67	18	17	24	71	22	69
5	8	54	55	57	12	58	59	49	4	50	51	65	20	66	67	69	72	22	71	13	64	62	15
6	55	5	56	58	11	9	12	2	3	49	4	18	19	65	20	22	23	21	72	62	15	61	16
7	6	8	5	11	10	12	57	3	50	52	49	67	18	20	17	71	22	24	21	63	62	16	13
8	53	55	6	60	57	11	58	52	49	51	2	20	17	19	66	72	21	71	70	64	61	63	62
9	11	12	58	49	3	4	50	5	7	8	54	69	23	72	22	13	15	16	62	17	67	20	18
10	60	11	9	2	52	3	49	6	8	55	5	22	24	23	21	62	16	63	61	66	20	19	17
11	57	58	60	51	49	2	4	55	5	54	56	23	21	70	72	15	61	62	64	67	65	66	20
12	10	57	11	52	50	49	51	8	54	53	55	72	22	21	71	64	62	13	63	68	66	17	67
13	63	62	16	21	71	22	72	17	67	66	20	49	3	2	52	57	11	10	60	53	55	6	8
14	16	13	15	22	24	69	71	18	68	17	67	50	4	49	3	10	12	9	11	6	8	5	7
15	13	64	62	71	69	72	70	67	65	68	66	51	49	52	50	59	57	12	10	7	53	8	54
16	62	15	61	72	22	23	69	20	18	67	65	4	2	51	40	12	58	11	57	8	54	55	5
17	66	20	19	61	62	16	15	21	22	72	23	5	6	56	55	49	2	52	51	57	58	60	11
18	17	67	20	62	13	15	64	22	69	71	72	54	5	55	8	50	49	3	52	10	57	11	12
19	20	18	65	15	16	14	13	23	24	22	69	7	56	54	5	3	4	2	49	11	12	58	9
20	67	66	66	64	15	61	14	72	23	69	70	56	55	53	54	4	51	49	50	12	59	57	58
21	72	23	70	65	20	19	18	61	16	15	14	9	60	59	58	5	56	55	54	49	4	51	2
22	71	72	21	66	67	20	65	62	15	64	61	58	11	60	57	54	55	8	53	50	51	52	49
23	22	69	72	67	18	65	68	15	14	13	64	59	58	57	12	7	54	5	8	3	50	49	4
24	21	22	23	20	17	18	67	16	13	62	15	12	9	58	11	8	5	6	55	52	49	2	3

[16]

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