Chapter 2

Treatment of Group Theory in Spectroscopy

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Abstract

The most important thing to consider when applying group theory is finding the molecule's point group or its particular symmetry operations. In order to identify a molecule's symmetry operations, one must first find the molecule's symmetry elements. In other words, the first stage in utilizing group theory with molecular properties is identifying a molecule's symmetry elements. For most beginners without experience this has proven to be most difficult because it requires the individual to visually identify the elements of symmetry in a 3D object. However, once this is overcome, applying group theory to forefront point groups and symmetry operations becomes second nature.

Keywords: group theory, symmetry operation, point group, spectroscopy, molecular energy levels

1. Introduction

Spectroscopy is defined as the scientific study of the many interactions between electromagnetic radiation and matter. Previously, spectroscopy came from the study of visible light that is dispersed with relation to its wavelength through a prism. As time progressed, the concept of spectroscopy was explored further and eventually included any interaction with energy derived from radiation that could be quantified and organized from its wavelength [1]. Max Planck's definition of blackbody radiation, Albert Einstein's view of the photoelectric effect, and Niels Bohr's understanding of atomic structure and spectra collectively come together to define spectroscopic studies and develop what is known as quantum. Spectroscopy is utilized constantly in both analytical and physical chemistry because unique spectra are found in atoms and molecules. Therefore, spectroscopy is utilized often to discover, define, and quantify information about the molecules and atoms. There are other fields that utilize spectroscopy as well such as astronomy, for remote sensing on Earth [2]. Spectroscopy is a sufficiently broad field that many subdisciplines exist, each with numerous implementations of specific spectroscopic techniques. The various implementations and techniques can be classified in several ways. Spectroscopy is a very wide field that has multiple subcategories, each with its own application of techniques unique to spectroscopy. The various implementations and techniques can be classified in several ways. A few examples of the multitude of spectroscopy categories are scanning tunneling microscopy spectroscopy (with Gerd Binnig and Heinrich Rohrer, 1981), electron paramagnetic resonance (with Yevgeny Zavoisky, 1944), nuclear magnetic resonance (with Edward Mills Purcell and Felix Bloch, 1940s), microwave spectroscopy (with James Clerk Maxwell, 1864), and infrared spectroscopy (with Sir Frederick William Herschel, 1800). These are also the most significant developments over the past three centuries [3].

This book chapter presents the treatment of group theory in spectroscopy. Group theory is a powerful formal method for analyzing abstract and physical systems in which symmetry is present and has surprising importance in physics, especially quantum mechanics. Gauss developed group theory but did not publish parts of its mathematics. Therefore, Galois is generally considered to have been the first to develop the theory. Group theory was developed in the nineteenth century and found its first remarkable applications in physics in the twentieth century by Bethe (1929), Wigner (1931), and Kohlrausch (1935). "*It is often hard or even impossible to obtain a solution to the Schrödinger equation - however, a large part of qualitative results can be obtained by group theory. Almost all the rules of spectroscopy follow from the symmetry of a problem*", said Eugene Wigner (1931). Groups are very important in most fields, but especially in physics, because they serve to illustrate the symmetries that the laws of physics obey as well. Continuous symmetry of a physical system directly relates to a conservation law of the system, according to Noether's theorem. This is why many physicists become interested in group representations, especially of Lie groups, because they often point the way to the potential physical theories that may define them. The usages of these groups in physics include the standard model, gauge theory, the Lorentz group, and the Poincare group [3]. Group theory is used in other areas of science such as in chemistry and materials science where groups are used to classify crystal structures, regular polyhedra, and the symmetries of molecules. The assigned point groups can then be used to determine physical and spectroscopic properties and to construct molecular orbitals. Molecular symmetry is responsible for many physical and spectroscopic properties of compounds and provides relevant information about how chemical reactions occur.

The group theory has also been extensively utilized in many areas such as statistical mechanics, music, and harmonic analysis. In statistical mechanics, group theory can be used to resolve the incompleteness of the statistical interpretations of mechanics developed by Willard Gibbs, relating to the summing of an infinite number of probabilities to yield a meaningful solution. In music, the presence of the 12-periodicity in the circle of fifths yields applications of elementary group theory. In harmonic analysis, Haar measures, which are integrals invariant under the translation in a Lie group, are used for pattern recognition and other image processing techniques. Due to the various applications of group theory, it has proven to be one of the most powerful mathematical tools utilized in the field of spectroscopy and in quantum chemistry. It provides opportunities for individuals to adequately understand the molecule and make informed inferences, which helps to break down complex theory and information. The most important understanding that this helps individuals to comprehend is that the set of operations associated with the symmetry elements of a molecule, collectively constitute a mathematical set called a group. What this serves to exemplify is that the application of mathematical theory can be applied when working with symmetry operations [4].

It is worth mentioning that the application of group theory in spectroscopy shed light on a molecule's symmetry that pertains to physical characteristics. This is effective when attempting to determine important physical data of a molecule. There are certain things that the symmetry of a molecule can help to deduce such as the energy levels that the orbitals will be at. Additionally, orbital symmetries in which unique transitions can occur between energy levels can also be determined. Bond order is also relatively easier to determine with tedious computation. The aforementioned examples place an emphasis on what makes group theory a very important tool [5].

2. Symmetry operations

Symmetry and group theory are intertwined in a multitude of ways. For instance, a symmetry group contains symmetry characteristics of common geometrical objects. The group contains the set of transformations that leave the object unchanged and the operation of combining two such transformations by performing one after the other. Lie groups are the symmetry groups used in the Standard Model of particle physics. Poincaré groups, which are also Lie groups, can express the physical symmetry underlying special relativity and point groups are also used to help understand symmetry phenomena in molecular chemistry [6].

2.1. Definition of a group

A group **G** is a finite or infinite set of elements together with a binary operation, that satisfy the four fundamental properties called the group axioms, namely, closure, associativity, identity, and invertibility [7].

2.1.1. Closure

For all elements A and B of the group G, we have

$$\mathbf{A}\,\mathbf{B}=\mathbf{C} \tag{1}$$

The result **C** is also an element of the group **G**.

2.1.2. Associativity

The combination rule must be associative, such that

$$\mathbf{A}\,(\mathbf{B}\,\mathbf{C})=(\mathbf{A}\,\mathbf{B})\,\mathbf{C} \tag{2}$$

2.1.3. Identity

There must be an element called the identity **I**, such that,

$$\mathbf{I\ R{=}R\ I{=}R} \tag{3}$$

This is true for all elements **R** of the group **G**.

2.1.4. Invertibility

Each element R must have an inverse R^{-1}, which is also a group element such that,

$$\mathbf{R\ R^{-1}{=}R^{-1}\ R{=}I} \tag{4}$$

A group is a "*monoid*" if each of its elements is invertible. Group theory is the study of groups. A group consisting of a fixed number of elements is known as a finite group, and the elements are defined as the group order of the group. A group may contain subgroups. The elements of a group that fall under group and inverse operations form a subgroup. Each subgroup is, in its turn, a group, and many known groups are, in fact, distinct subgroups of larger groups. The symmetric group $\mathbf{S_n}$ is a classic example of a finite group, while integers subjected to addition are a basic example of an infinite group. For continuous groups, one can consider the real numbers or the set of **n x n** invertible matrices [8]. The most well-known group is that of integers subjected to addition, though the theoretical formalization of the group axioms applies more widely if taken separately from the characteristics of any group and its governing operation. It allows entities with highly diverse mathematical origins in abstract algebra and beyond to be handled in a flexible way while retaining their essential structural aspects. The ubiquity of groups in numerous areas within and outside mathematics makes them a central organizing principle of contemporary mathematics [2]. The concept of a group arose from the study of polynomial equations, starting with Evariste Galois in the 1830s. After contributions from other fields such as number theory and geometry, the group notion was generalized and firmly established around 1870.

In group theory, the elements considered are symmetry operations. For a given molecular system described by the Hamiltonian $\boldsymbol{H}$, there is a set of symmetry operations $\boldsymbol{O_i}$, which commute with the Hamiltonian $\boldsymbol{H}$. $\boldsymbol{H}$ and $\boldsymbol{O_i}$ thus have a common set of Eigen functions, and the eigenvalues of $\boldsymbol{O_i}$ can be used as labels for the Eigen functions. This set of operations defines a symmetry group. In molecular physics and molecular spectroscopy, two types of groups are particularly important: the point groups and the permutation-inversion groups.

2.2. Point group operations and point group symmetry

Each molecule has a set of symmetry operations that describes the molecule's overall symmetry. This set of operations defines the point group of the molecule. Since all the elements of symmetry present in the molecule intersect at a common point, this point remains fixed under all symmetry operations of the molecule and is known as point symmetry groups. **Table 1** highlights the Common Point Groups and Symmetry Elements [9]. The point groups are utilized to define molecules that are considered to be rigid when observed through the timescale of the particular spectroscopic experiment. Therefore, molecules that have a specific equilibrium configuration with no observable tunneling between two or more similar configurations can be used to define the point groups. There are five key symmetry operations for point groups. The first is the identity E, which leaves all coordinates unaltered. Next is the rotation C_n by an angle of $2\pi/n$ in the positive trigonometric sense. The symmetry axis with the greatest n value is chosen as the principal axis. If a molecule has a specific C_n axis with the greatest n value, then the molecule has a sustained dipole moment that lies along this axis. If a molecule has several C_n axes with the greatest n value, the molecule has no permanent dipole moment. The reflection through a plane is the next important key factor. These reflections are organized into two main categories. The first is a reflection through a horizontal plane, and the second the reflection through a vertical plane. Next on the list of key factors is the inversion, typically represented by (i), of all coordinates through the inversion center. Through this inversion, we discover the need for the next key factor for symmetry operation, which is the improper rotation, typically denoted as "S_n" or referred to as "*rotation-reflection*", which consists of a rotation by an angle of $2\pi/n$ around the z-axis, followed by a reflection through the plane perpendicular to the rotational axis. A molecule having an improper operation as symmetry operation is not able to be optically active and is subsequently labeled as achiral, as opposed to chiral. One example of symmetry is found within stereochemistry, more specifically, isomeric pairs of molecules called enantiomers. Enantiomers are mirror images of each

Point group	Symmetry elements	Simple description, chiral if applicable	Illustrative species
C_1	E	No symmetry, chiral	CFIBrH, Lysergic acid
C_8	E σ_h	Planar, no other symmetry	Thionyl chloride, hypochlorous acid
C_i	E_i	Inversion center	Anti 1,2-dichloro-1,2-dibromoethane
$C_\infty v$	E_2C_∞ σ_v	Linear	Hydrogen chloride, carbon monoxide
$D_{\infty h}$	E_2C_∞ $\infty\sigma_i$ i $2S_\infty$ ∞C_2	Linear with inversion center	Dihydrogen, azide anion, carbon dioxide
C_2	EC_2	"open book geometry," chiral	Hydrogen peroxide
C_3	EC_3	Propeller, chiral	Triphenylphosphine
C_{2h}	E C_2 i σ_h	Planar with inversion center	Trans-1,2- dichloroethylene
C_{3h}	$EC_3C_3^2$ σ_h $S_3S_3^5$	Propeller	Boric acid
C_{2v}	E C_2 $\sigma_v(xz)$ $\sigma_v'(yz)$	Angular (H_2O) or see-saw (SF_4)	Water, sulfur tetrafluoride, sulfuryl fluoride
C_{3v}	$E_2C^3 3\sigma_v$	Trigonal pyramidal	Ammonia, phosphorus oxychloride
C_{4v}	$E_2C_4C_2 2\sigma_v$ $2\sigma_d$	Square pyramidal	Xenon oxytetrafluoride
T_d	$E_8C_3 3C_2 6S_4 6\sigma_d$	Tetrahedral	Methane, phosphorus pentoxide. Adamantine
O_h	E $8C_3$ $6C_2$ $6C_4$ $3C_2$ i $6S_4$ $8S_6$ $3\sigma_h$ $6\sigma_d$	Octahedral or cubic	Cubane, sulfur hexafluoride
I_h	E $12C_5$ $12C_5^2$ $20C_3$ $15C_2$ i $12S_{10}$ $12S_{10}^3$ $20S_6$ 15σ	Icosahedral	C_{60}, $B_{12}H_{12}^{2-}$

Table 1. Common point groups and symmetry elements.

other, but, when superimposed, the images are not identical. A consequence of this symmetrical relation is that they rotate the plane of polarized light passing through them in opposite directions. Molecules that fit this description are referred to as chiral. These aforementioned applications help to mitigate tedious research timescales and also place an emphasis on the symmetrical allocation to specific molecules and molecular geometry shapes.

2.3. Permutation-inversion operations and CNPI groups

The point groups are appropriated to describe rigid molecules. However, for floppy systems or when the transition between two states does not hold the same symmetry, another, more general definition is required. Longuet-Higgins and Hougen developed the complete nuclear permutation-inversion (CNPI) groups that rely on the fact that the symmetry operations leave the Hamiltonian unaltered. There are several symmetry operations of the CNPI groups. The first is the permuation (ij) of the coordinates of two identical nuclei. i and j denote the exchange of the nucleus i with the nucleus j [7]. The second is the cyclic permutation (ijk) of the coordinates of three identical nuclei i, j, and k. The nucleus i is replaced by the nucleus j, j by k, and k by i. We have all possible circular permutations of n identical nuclei. Next we have the inversion E^* of all coordinates of all particles through the center of the lab-fixed frame. We also have the permutation followed by an inversion $(ij)^* = E{*}\cdot(ij)$ of all coordinates of all particles and the cyclic permutation followed by an inversion $(ijk)^*$ of all coordinates of all particles. Finally, we have all possible circular permutations followed by an inversion of all coordinates of n identical nuclei. The molecular Hamiltonian is left unchanged upon these operations because the permutation operations affect identical nuclei. The CNPI groups represent a more general description that can also be applied to rigid molecules. The point groups are commonly used in the case of rigid molecules. In the following, we will consider only rigid molecules and restrict ourselves to point group symmetry, but all concepts can be extended to the CNPI and MS groups [7]. The key to applying group theory is to be able to identify the point group of the molecule that describes the molecule's unique collection of symmetry operations. The symmetry elements of a molecule reveal the molecule's various symmetry operations. Thus, the initial step in applying group theory to molecular properties is to recognize the molecule's specific set of symmetry elements. The process of identifying a molecule's symmetry elements has proven difficult for beginners, as they must observe the elements of symmetry with the naked eye in a 3D object [4].

3. Applications of group theory in spectroscopy

Symmetry can help to solve many of the issues encountered in chemistry, and group theory is the primary tool that is utilized to identify symmetry. If we know how to determine the symmetry of small molecules, we can determine the symmetry of other targets. This is not only limited to the symmetry of molecules but also to the symmetries of local atoms, molecular orbitals, rotations, and vibrations of bonds. A typical example is the knowledge of the symmetries of molecular orbital wave functions allowing the identification of the nature and characteristics of the binding. Also, the particular methods associated with certain symmetries allow us to decide if the transition is prohibited and to understand the bands observed in infrared or Raman spectrum. A *symmetry operation* to a molecule is an operation that leaves the physical proprieties of the molecule unchanged. This is equivalent to having the molecule unchanged before and after the symmetry operation is performed [5]. In other words, when we do a symmetry operation on a molecule, every point of the molecule will be in an equivalent position.

The application of group theory in spectroscopy intends to investigate the way in which symmetry considerations influence the interaction of light with matter. Group theory can be used to understand the molecular orbitals in a molecule and to determine the possible electronic states accessible by absorption of a photon. Another important function of group theory is the investigation of the light that excites different vibrational modes of a polyatomic molecule [10]. A photon of the appropriate energy is able to excite an electronic transition in an atom, subject to the following selection rules:

$$\Delta n = Integer \tag{5}$$

$$\Delta l = \pm 1 \tag{6}$$

$$\Delta L = 0, \pm 1 \tag{7}$$

$$\Delta S = 0 \tag{8}$$

$$\triangle J = 0, \pm 1; J = 0 \tag{9}$$

In general, different types of spectroscopic transitions obey different selection rules. The common transitions involve changing the electronic state of an atom and involve absorption of a photon in the UV or visible part of the electromagnetic spectrum. There are analogous electronic transitions in molecules, which we will consider here. The absorption of photons in the infrared region of the spectrum controls the vibrational excitation in molecules and the absorption of photons in the microwave region commands rotational excitation. Typically, each excitation executes its own selection rules, but the general methodology for establishing the selection rules is identical in all cases. The determination of the conditions under which the probability of transition is not zero is a simple process. Therefore, the first step in understanding the origins of selection rules is to learn how transition probabilities are computed, and this requires some quantum mechanics concepts [10]. Overall, group theory plays a very important role in spectroscopy, which we can see from various applications of group theory in spectroscopy such as infrared spectrum, Raman spectrum, electronic spectrum, and so on. Typically, the change in electronic energy is greater than in vibrational energy, which is also greater than in rotational energy. **Figure 1** illustrates the different energy levels in a molecule.

3.1. Electronic transitions in molecules

When an electron is excited from one electronic state to another, this is what is called an electronic transition. The selection rules for electronic transitions are governed by the transition moment integral. Due to the fact that the electrons are coupled between two vibrational states that are between two electronic states, it is important to consider both the electronic state

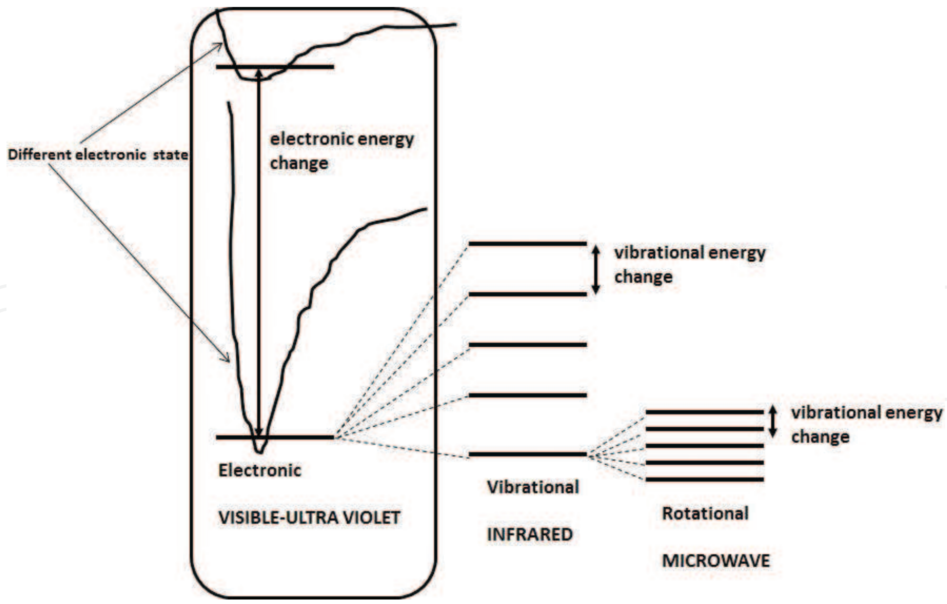

Figure 1. Molecular energy levels diagram.

symmetries and the vibration state symmetries. This modification of the transition moment integral produces the symmetry of the initial electronic and vibrational states called "***bra***" and the final electronic and vibrational states named "***ket.***"

This appears to be a modified version of the transition moment integral [5]. If we assume that we have a molecule in an initial state, we can determine which final states can be accessed by the absorption of a photon. So, we need to determine the symmetry of an electronic state. The symmetry of an electronic state is obtained by identifying any unpaired electrons and taking the direct product of the unrepresentative of the molecular orbitals in which they are detected. The total symmetric unrepresentative always holds the ground state of a closed-shell molecule in which all electrons are paired [10]. The determination of the unrepresentative electric dipole operator allows obtaining the electronic states accessible by absorption of photons. Light that is linearly polarized along the x, y, and z axes transforms in the same way as the functions x, y, and z in the appropriate character table. From the $\mathbf{C_{3v}}$ character table, we see that x- and y-polarized light transforms as **E**, while z-polarized light transforms as in the appropriate character table [10].

The excitation from one energy level to a higher energy level happens during the electronic transitions in a molecule. The change of energy associated with these transitions gives structural information of the molecule and determines many other molecular properties such as color. Planck's relation provides the relationship between the energy involved in the electronic transition and the frequency of radiation. Planck's equation is sometimes termed the Planck-Einstein:

$$E = h\gamma \tag{10}$$

where $h = 6.55 \times 10^{-34} J.s$ is a Planck constant. Electronic transitions in molecules occur between orbitals and they must cohere to angular momentum selection rules. **Figure 2** shows possible *electronic* transitions of p, s, and n electrons. In the process of transition $\sigma \rightarrow \sigma^*$, electrons occupying a "HOMO" of a "sigma bond" can get excited to the "LUMO" of that bond. Similarly, in the process of transition $\pi \rightarrow \pi^*$, electrons from a "pi-bonding orbital" can get excited to the "antibonding-pi orbital" of that bond. Auxochromes with free electron pairs denoted as n have their own transitions. The following molecular electronic transitions exist:

3.2. Vibrational transitions in molecules

All molecules vibrate. While these vibrations can originate from several events, the most basic of these occurs when an electron is excited within the electronic state from one eigenstate to another. When an electron is excited from one eigenstate to another within the electronic state, there is a change in interatomic distance, which results in a vibration occurring. A vibration occurs when an electron remains within the electronic state but changes from one eigenstate to another. Just as in electronic transitions, the selection rules for Vibrational transitions are dictated by the transition moment integral. Light polarized along the x, y, and z axes of the molecule may be used to excite vibrations with the same symmetry as the x, y, and z functions listed in the character table. For example, in the $\mathbf{C_{2v}}$ point group, x-polarized light may be used to excite vibrations of $\mathbf{B_1}$ symmetry, y-polarized light to excite vibrations of $\mathbf{B_2}$ symmetry, and z-polarized light to excite vibrations of $\mathbf{A_1}$ symmetry. In $\mathbf{H_2O}$, we would use z-polarized light to excite the symmetric stretch and bending modes, and x-polarized light to excite the asymmetric stretch. Shining y-polarized light onto a molecule of $\mathbf{H_2O}$ would not excite any vibrational motion [10]. For instance, let us consider a simple case of a vibrating diatomic molecule where the restoring force is proportional to the displacement,

$$F = -kx. \tag{11}$$

The potential energy is

$$V = \frac{1}{2}kx^2 \tag{12}$$

and the allowed energy can be obtained from Schrodinger equation,

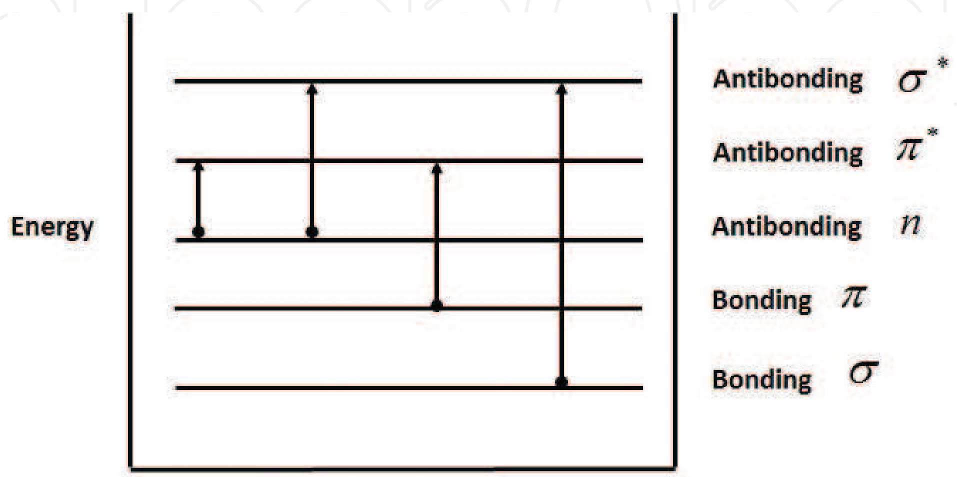

Figure 2. Absorbing species containing p, s, and n electrons.

$$E_\nu = \left(\nu + \frac{1}{2}\right)\hbar\omega \tag{13}$$

where

$$\omega = \left(\frac{k}{\mu}\right)^{1/2}, \nu = 0, 1, 2, 3, 4\ldots, \tag{14}$$

and

$$\mu = \frac{m_1 m_2}{m_1 + m_2}. \tag{15}$$

The vibrational terms of the molecule can therefore be given by

$$G_\nu = \left(\nu + \frac{1}{2}\right)\frac{1}{2\pi c}\left(\frac{k}{\mu}\right)^{1/2} \tag{16}$$

3.3. Raman scattering

Single photons often cannot reach vibrational modes in the molecule; however, it may still be possible to excite them. To achieve excitement, scientists often utilize Raman scattering, which is a two-photon process. These two photons utilized in Raman scattering might have different polarizations. The first photon sends the molecule into an intermediate state known as a virtual state, which is not a stationary state for the particular molecule. When considering the photon and the molecule as a system, a stationary state can be said to exist, but it exists only for a short period of time. Once the transition is over, a photon will be rapidly emitted back into the stable molecule. It is important to note that the photon may return different from its original state. The transition dipole for a particular Raman transition transforms as one of the Cartesian products. A Raman transition has the potential to excite Cartesian products if they are the product of a transformed vibrational mode. For example, modes that transform as x, y or z can be excited by a one-photon vibrational transition. Simple one-photon vibrational transitions can access all of the vibrational modes of water Raman transitions). The Cartesian products transform as follows in the $\mathbf{C_{2v}}$ point group. The stretch and the bending vibration of water are depictions of $\mathbf{A_1}$ symmetry. Consequently, Raman scattering processes involving two photons of identical polarization (x-, y- or z-polarized) can excite both. Conversely, an asymmetric stretch can be excited if one photon is x-polarized and the other is z-polarized.

As shown in **Figure 3**, Raman spectroscopy transition in resonance is the excitation from one particular electronic state to another state. The rules for selection are determined by the transition moment integral discussed in the electronic spectroscopy segment. Mechanically, Raman does produce a vibration similar to infrared, but selection protocols for Raman state that there must be a change in the polarization, which means that the volume occupied by the molecule must change [5]. The utilization of group theory to identify whether or not a transition is permitted can also be done using the transition moment integral presented in the electronic transition portion.

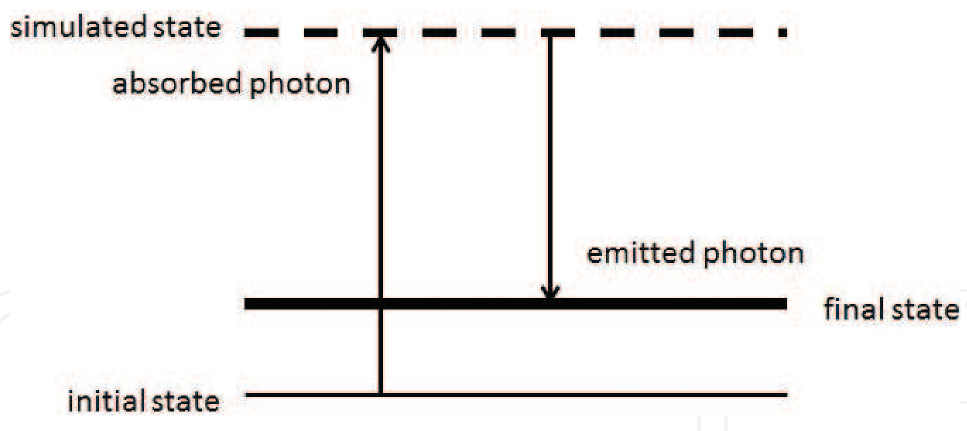

Figure 3. Raman scattering energy level diagram.

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