

Selection Rules

A **selection rule** is a rule that states how the probability of transitioning from one level to another cannot be **zero**. It has two sub-pieces: a **gross selection rule** and a **specific selection rule**. A gross selection rule illustrates characteristic requirements for atoms or molecules to display a spectrum of a given kind, such as an IR spectroscopy or a microwave spectroscopy. Once the atom or molecules follow the gross selection rule, the specific selection rule must be applied to the atom or molecules to determine whether a certain transition in quantum number may happen or not.

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Background

The **transition dipole moment** is the product of **radial function**, $R(r)$, and **spherical harmonics**, $Y(\theta, \phi)$. The transition dipole moment is also equal to probability of transitioning when it is squared.

$$\mu_{ij} = R(r)Y(\theta, \phi)$$

n , principal quantum #

m magnetic q. number

Where i is the initial quantum number, j is the final quantum number and μ_{ij} is the transition dipole moment. Usually, the radial functions exist respect to n (principal quantum number) and spheric harmonics functions exist respect to m (magnetic quantum number). Many types of selection rules exist, such as the selection rules for angular momentum, central force problems, Harmonic Oscillator, and spin.

Selection Rule for Angular Momentum

m before n

$$\Delta m = \pm 1, 0$$

For **angular momentum**, m have to be considered first before n . Then the selection rule can be applied to atoms or to a rotational spectroscopy. After finding an expression for the μ_{ij} and squaring it, which is the probability of transitioning from state i to state j , the probability will be **zero** unless $m_i = m_j + 1$, $m_j = m_i - 1$, or $m_i = m_j$. Therefore, the **selection rule for the angular momentum** is $\Delta m = \pm 1, 0$.

Selection Rule for Central Force Problems: Hydrogen Atom

n can be anything $i/3$

The electric dipole moment must change in the course of vibration motion.

can be from zero to non-zero

* At room temperature only the "fundamental transition" of vibration is seen from $v=0$ to $v=1$.

* There is always one single line in the spectrum. $\Delta v = \pm 1$

* Deviation from $\Delta v = \pm 1$ is observed. $\Delta v = \pm 2$ may be observed.

For **central force problems**, n has to be considered then applied to atoms or to spectroscopy. After finding an integrated expression for a radial function and square it, the probability will exist no matter what the value of n is as long as n is an integer greater than zero. Therefore, for central force problems, the selection rule is that n can be any positive integer starting from 1.

$$n = 1, 2, 3, \dots$$

Selection Rule for Harmonic Oscillator

$$\Delta n = \pm 1$$

For the **harmonic Oscillator**, n has to be considered for the selection rule, then apply it to atoms or a spectroscopy (definition). After finding a radial function and square it, n will be **zero** unless $n = \pm 1$. Therefore, $n = \Delta \pm 1$ is the selection rule for the harmonic oscillator.



Selection Rules based on Spin

Same spin $\Delta S = 0$ if Hamiltonian is spin independent.

When the Hamiltonian of a system is spin **independent**, the system in transitions that are allowed must have the **same spin**. However, if the Hamiltonian is spin dependent, then this selection rule can not be applied.

References

1. Anderson, J.M. Introduction to Quantum Chemistry, 1969, W.A. Benjamin, Inc, pg.259-263.
2. Atkins, Peter and de Paula, Julio. Physical Chemistry for the Life Sciences. New York: W.H. Freeman and Company. p. 548.

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Rotational Spectroscopy of Diatomic Molecules

The rotation of a diatomic molecule can be described by the **rigid rotor** model. To imagine this model think of a spinning dumbbell. The dumbbell has two masses set at a fixed distance from one another and spins around its center of mass (COM). This model can be further simplified using the concept of reduced mass which allows the problem to be treated as a single body system.

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Introduction

Similar to most quantum mechanical systems our model can be completely described by its wave function. Therefore, when we attempt to solve for the energy we are lead to the Schrödinger Equation. In the context of the rigid rotor where there is a natural center (rotation around the COM) the wave functions are best described in spherical coordinates. In addition to having pure rotational spectra diatomic molecules have rotational spectra associated with their vibrational spectra. The order of magnitude differs greatly between the two with the rotational transitions having energy proportional to $1\text{-}10\text{ cm}^{-1}$ (microwave radiation) and the vibrational transitions having energy proportional to $100\text{-}3,000\text{ cm}^{-1}$ (infrared radiation). Rotational spectroscopy is therefore referred to as microwave spectroscopy.

Rigid Rotor Model

A diatomic molecule consists of two masses bound together. The distance between the masses, or the bond length, (l) can be considered fixed because the level of vibration in the bond is small compared to the bond length. As the molecule rotates it does so around its COM (observed in Figure 1. as the intersection of R1 and R2) with a frequency of rotation of ν_{rot} given in radians per second.

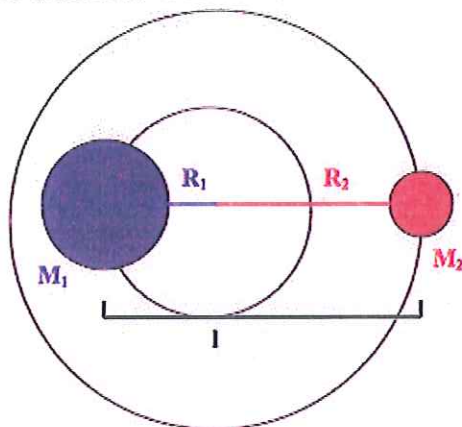


Figure 1. Rigid Rotor Model of a Diatomic Molecule

Reduced Mass

The system can be simplified using the concept of reduced mass which allows it to be treated as one rotating body.

1.) The system can be entirely described by the fixed distance between the two masses instead of their individual radii of rotation. Relationships between the radii of rotation and bond length are derived from the COM given by: $M_1R_1 = M_2R_2$, where l is the sum of the two radii of rotation: $l = R_1 + R_2$.

2.) Through simple algebra both radii can be found in terms of their masses and bond length:
 $R_1 = \frac{M_2}{M_1 + M_2}l$ and $R_2 = \frac{M_1}{M_1 + M_2}l$.

3.) The kinetic energy of the system, T , is sum of the kinetic energy for each mass:
 $T = \frac{M_1v_1^2 + M_2v_2^2}{2}$, where $v_1 = 2\pi R_1\nu_{rot}$ and $v_2 = 2\pi R_2\nu_{rot}$.

4.) Using the angular velocity, $\omega = 2\pi\nu_{rot}$, the kinetic energy can now be written as:
 $T = \frac{M_1R_1^2 + M_2R_2^2}{2}\omega^2$.

5.) With the moment of inertia, $I = M_1R_1^2 + M_2R_2^2$, the kinetic energy can be further simplified:
 $T = \frac{I\omega^2}{2}$.

6.) The moment of inertia can be rewritten by plugging in for R_1 and R_2 : $I = \frac{M_1M_2}{M_1 + M_2}l^2$, where $\frac{M_1M_2}{M_1 + M_2}$ is the reduced mass, μ .

7.) The moment of inertia and the system are now solely defined by a single mass, μ , and a single length, l : $I = \mu l^2$.

Angular Momentum

Another important concept when dealing with rotating systems is the angular momentum defined by: $L = I\omega$

Looking back at the kinetic energy: $T = \frac{I\omega^2}{2} = \frac{I^2\omega^2}{2I} = \frac{L^2}{2I}$

The angular momentum can now be described in terms of the moment of inertia and kinetic energy: $L^2 = 2IT$.

Setting up the Schrodinger Equation

1.) The wave functions for the rigid rotor model are found from solving the Schrodinger Equation:

$$\hat{H}\psi = E\psi$$

2.) Where the Hamiltonian Operator is: $\hat{H} = \frac{-\hbar^2}{2\mu} \nabla^2 + V(r)$

∇^2 is known as the Laplacian Operator and can be represented in either cartesian coordinates:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

or in spherical coordinates:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

At this point it is important to incorporate two assumptions:

a.) The distance between the two masses is fixed. This causes the terms in the Laplacian containing $\frac{\partial}{\partial r}$ to be zero.

b.) The orientation of the masses is completely described by θ and ϕ and in the absence of electric or magnetic fields the energy is independent of orientation. This causes the potential energy portion of the Hamiltonian to be zero.

The wave functions $\psi(\theta, \phi)$ are customarily represented by $Y(\theta, \phi)$ and are called spherical harmonics.

3.) The Hamiltonian Operator can now be written: $\hat{H} = \hat{T} = \frac{-\hbar^2}{2\mu l^2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$

With the Angular Momentum Operator being defined:

a.) $\hat{L} = 2I\hat{T}$

$$b.) \hat{L} = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$$

4.) And the Schrodinger Equation now expressed:

$$\frac{-\hbar^2}{2I} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] Y(\theta, \phi) = EY(\theta, \phi)$$

Solving the Schrodinger Equation

The Schrodinger Equation can be solved using separation of variables.

1.) Let, $Y(\theta, \phi) = \Theta(\theta)\Phi(\phi)$, and substitute: $\beta = \frac{2IE}{\hbar^2}$.

2.) Set the Schrodinger Equation equal to zero: $\frac{\sin \theta}{\Theta(\theta)} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \beta \sin^2 \theta + \frac{1}{\Phi(\phi)} \frac{d^2 \Phi}{d\phi^2} = 0$

3.) Because the terms containing $\Theta(\theta)$ are equal to the terms containing $\Phi(\phi)$ they must equal the same constant in order to be defined for all values:

$$a.) \frac{\sin \theta}{\Theta(\theta)} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \beta \sin^2 \theta = m^2$$

$$b.) \frac{1}{\Phi(\phi)} \frac{d^2 \Phi}{d\phi^2} = -m^2$$

3.) Solving for Φ is fairly simple and yields:

$$a.) \Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}, \text{ where } m = 0, \pm 1, \pm 2, \dots$$

Solving for θ is considerably more complicated but gives the quantized result:

$$b.) \beta = J(J+1), \text{ where } J \text{ is the rotational level and } J=0, 1, 2, \dots$$

4.) The energy is quantized by expressing in terms of β : $E = \frac{\hbar^2 \beta}{2I}$

5.) Using the rotational constant, $B = \frac{\hbar^2}{2I}$, the energy is further simplified: $E = BJ(J+1)$

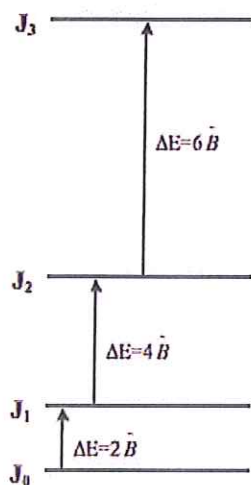
Energy of Rotational Transitions

When a molecule is irradiated with photons of light it may absorb the radiation and undergo an energy transition. The energy of the transition must be equivalent to the energy of the photon of light absorbed given by: $E = h\nu$. For a diatomic molecule the energy difference between rotational levels (J to $J+1$) is given by:

$$E_{J+1} - E_J = B(J+1)(J+2) - BJ(J+1) = 2B(J+1)$$

with $J=0, 1, 2, \dots$

Because the difference of energy between rotational levels is in the microwave region ($1-10 \text{ cm}^{-1}$) rotational spectroscopy is commonly called microwave spectroscopy. In spectroscopy it is customary to represent energy in wave numbers (cm^{-1}), in this notation B is written as \tilde{B} . To convert from units of energy to wave numbers simply divide by h and c , where c is the speed of light in cm/s ($c=2.998 \times 10^{10} \text{ cm/s}$). In wave numbers $\tilde{B} = \frac{h}{8\pi c I}$.



$$B = \frac{h^2}{2I}$$

$$I \uparrow \quad B \downarrow \quad \Delta E \downarrow$$

$$\Delta E = 2B(J+1)$$

Figure 2. Rotational Energy Levels

Figure 2 predicts the rotational spectra of a diatomic molecule to have several peaks spaced by $2\tilde{B}$. This contrasts vibrational spectra which have only one fundamental peak for each vibrational mode.

From the rotational spectrum of a diatomic molecule the bond length can be determined. Because \tilde{B} is a function of I and therefore a function of l (bond length), l is readily solved for:

$$l = \sqrt{\frac{h}{8\pi^2 c \tilde{B} \mu}}$$

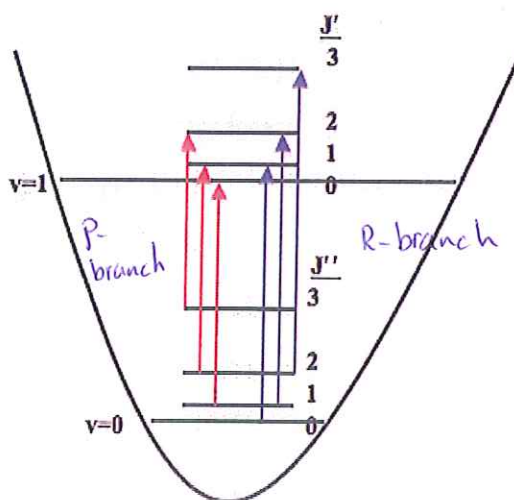
Note: Selection rules only permit transitions between consecutive rotational levels: $\Delta J = J \pm 1$, and require the molecule to contain a permanent dipole moment. Due to the dipole requirement, molecules such as HF and HCl have pure rotational spectra and molecules such as H_2 and N_2 are rotationally inactive.

Centrifugal Distortion \rightarrow higher speed at higher levels \Rightarrow reduce spacing between the levels.

As molecules are excited to higher rotational energies they spin at a faster rate. The faster rate of spin increases the centrifugal force pushing outward on the molecules resulting in a longer average bond length. Looking back, B and l are inversely related. Therefore the addition of centrifugal distortion at higher rotational levels decreases the spacing between rotational levels. The correction for the centrifugal distortion may be found through perturbation theory: $E_J = \tilde{B}J(J+1) - \tilde{D}J^2(J+1)^2$.

Rotation-Vibration Transitions

Rotational transitions are on the order of $1-10 \text{ cm}^{-1}$, while vibrational transitions are on the order of 1000 cm^{-1} . The difference of magnitude between the energy transitions allow rotational levels to be superimposed within vibrational levels.



Rotation $1-10 \text{ cm}^{-1}$
Vibration 1000 cm^{-1}

Figure 3. Rotation-Vibration Transitions

Combining the energy of the rotational levels, $\tilde{E}_J = \tilde{B}J(J+1)$, with the vibrational levels, $\tilde{E}_v = \tilde{\omega}(v+1/2)$, yields the total energy of the respective rotation-vibration levels: $\tilde{E}_{v,J} = \tilde{\omega}(v+1/2) + \tilde{B}J(J+1)$.

Following the selection rule, $\Delta J = J \pm 1$, Figure 3. shows all of the allowed transitions for the first three rotational states, where J'' is the initial state and J' is the final state.

When the $\Delta J = +1$ transitions are considered (blue transitions) the initial energy is given by: $\tilde{E}_{0,J} = \tilde{\omega}(1/2) + \tilde{B}J(J+1)$ and the final energy is given by: $\tilde{E}_{1,J+1} = \tilde{\omega}(3/2) + \tilde{B}(J+1)(J+2)$.

*The energy of the transition, $\Delta\tilde{\nu} = \tilde{E}_{1,J+1} - \tilde{E}_{0,J}$, is therefore: $\Delta\tilde{\nu} = \tilde{\omega} + 2\tilde{B}(J+1)$ where $J''=0, 1, 2, \dots$

When the $\Delta J = -1$ transitions are considered (red transitions) the initial energy is given by: $\tilde{E}_{v,J} = \tilde{\omega}(1/2) + \tilde{B}J(J+1)$ and the final energy is given by: $\tilde{E}_{v,J-1} = \tilde{\omega}(3/2) + \tilde{B}(J-1)J$.

*The energy of the transition is therefore: $\Delta\tilde{\nu} = \tilde{\omega} - 2\tilde{B}J$ where $J''=1, 2, 3, \dots$

The difference in energy between the $J+1$ transitions and $J-1$ transitions causes splitting of vibrational spectra into two branches. The $J-1$ transitions, shown by the red lines in Figure 3., are lower in energy than the pure vibrational transition and form the P-branch. The $J+1$ transitions, shown by the blue lines in Figure 3. are higher in energy than the pure vibrational transition and form the R-branch. Notice that because the $\Delta J = 0$ transition is forbidden there is no spectral line associated with the pure vibrational transition. Therefore there is a gap between the P-branch and R-branch, known as the q branch.

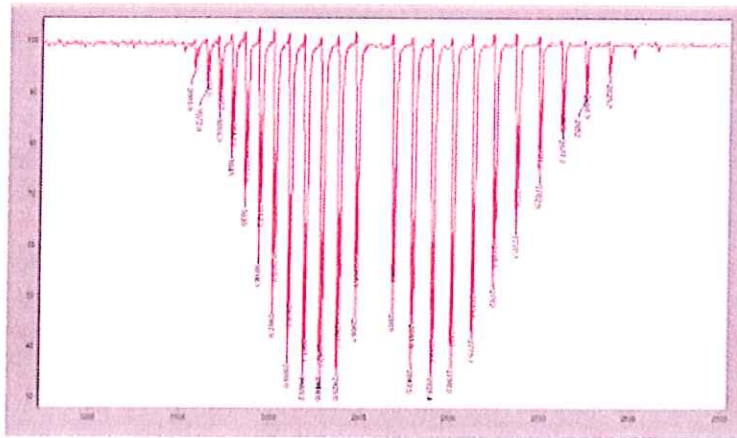


Figure 4. HCl Rotation-Vibration Spectrum

In the high resolution HCl rotation-vibration spectrum the splitting of the P-branch and R-branch is clearly visible. Due to the small spacing between rotational levels high resolution spectrophotometers are required to distinguish the rotational transitions.

Rotation-Vibration Interaction

Recall the Rigid-Rotor assumption that the bond length between two atoms in a diatomic molecule is fixed. However, the anharmonicity correction for the harmonic oscillator predicts the gaps between energy levels to decrease and the equilibrium bond length to increase as higher vibrational levels are accessed. Due to the relationship between the rotational constant and bond length:

$$\tilde{B} = \frac{h}{8\pi^2 c \mu l^2}$$

$r \uparrow \quad B \downarrow$

$$\tilde{B}_v = \tilde{B} - \tilde{\alpha} \left(v + \frac{1}{2} \right)$$

$B_v < B$

The rotational constant is dependent on the vibrational level:

Where $\tilde{\alpha}$ is the anharmonicity correction and v is the vibrational level.

anharmonicity correction

As a consequence the spacing between rotational levels decreases at higher vibrational levels and unequal spacing between rotational levels in rotation-vibration spectra occurs.

Including the rotation-vibration interaction the spectra can be predicted.

For the R-branch:

$$\tilde{E}_{1,J+1} - \tilde{E}_{0,J}$$

$B_1 < B_0$

instead of $2B(J+1) + w$

$$\tilde{\nu} = \left[\tilde{w} \left(\frac{3}{2} \right) + \tilde{B}_1 (J+1)(J+2) \right] - \left[\tilde{w} \left(\frac{1}{2} \right) + \tilde{B}_0 J(J+1) \right]$$

$$\tilde{\nu} = \tilde{w} + (\tilde{B}_1 - \tilde{B}_0) J^2 + (3\tilde{B}_1 - \tilde{B}_0) J + 2\tilde{B}_1 \quad \text{where } J=0, 1, 2, \dots$$

For the P-branch:

$$\tilde{E}_{1,J-1} - \tilde{E}_{0,J}$$

$$\tilde{\nu} = \left[\tilde{w} \left(\frac{3}{2} \right) + \tilde{B}_1 (J-1)J \right] - \left[\tilde{w} \left(\frac{1}{2} \right) + \tilde{B}_0 J(J+1) \right]$$

$$\tilde{\nu} = \tilde{w} + \underbrace{(\tilde{B}_1 - \tilde{B}_0)}_{\ominus} J^2 - (\tilde{B}_1 + \tilde{B}_0) J \quad \text{where } J=1, 2, 3, \dots \quad \text{instead of } w - 2BJ$$

Because $\tilde{B}_1 < \tilde{B}_0$,

As J increases:

- Spacing in the R-branch decreases.
- Spacing in the P-branch increases.

References

1. McQuarrie, Donald A. Quantum Chemistry. New York: University Science Books, 2007.

Outside Links

- [Wikipedia-SchrodingerEquation](#)
- [Wikipedia-RotationalSpectroscopy](#)
- [Wikipedia-InfraredSpectroscopy](#)
- [Wikipedia-CentrifugalForce](#)

Problems

1. What is the potential energy of the Rigid-Rotor?
2. Derive the Schrodinger Equation for the Rigid-Rotor.
3. Researchers have been interested in knowing what Godzilla uses as the fuel source for his fire breathing. A recent breakthrough was made and some residue containing Godzilla's non-combusted fuel was recovered. Studies on the residue showed that the fuel, Compound G, is a diatomic molecule and has a reduced mass of 1.615×10^{-27} kg. In addition, a microwave spectrum of Compound G was obtained and revealed equally spaced lines separated by 4.33 cm^{-1} . Using the Rigid-Rotor model determine the bond length of Compound G.
4. How would deuterium substitution effect the pure rotational spectrum of HCl?

Contributors

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Infrared Spectroscopy

Infrared Spectroscopy is the analysis of infrared light interacting with a molecule. This can be analyzed in three ways by measuring absorption, emission and reflection. The main use of this technique is in organic and inorganic chemistry. It is used by chemists to determine functional groups in molecules. IR Spectroscopy measures the vibrations of atoms, and based on this it is possible to determine the functional groups.⁵ Generally, stronger bonds and light atoms will vibrate at a high stretching frequency (wavenumber).

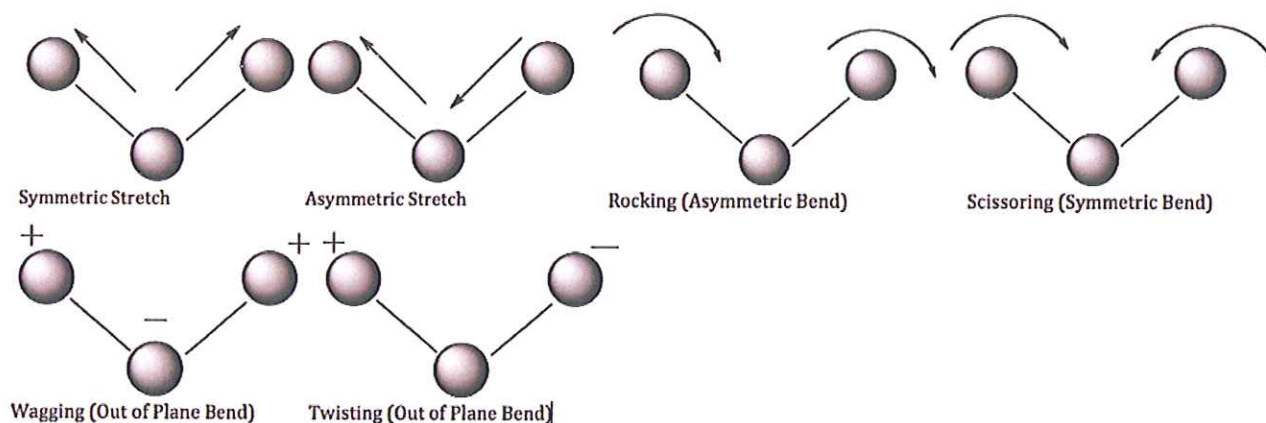
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Introduction

The use of infrared spectroscopy began in the 1950's by Wilbur Kaye. He had designed a machine that tested the near-infrared spectrum and provided the theory to describe the results. Karl Norris started using IR Spectroscopy in the analytical world in the 1960's and as a result IR Spectroscopy became an accepted technique. There have been many advances in the field of IR Spec, the most notable was the application of Fourier Transformations to this technique thus creating an IR method that had higher resolution and a decrease in noise. The year this method became accepted in the field was in the late 1960's.⁴

Theory

Infrared light imposed on a molecule will not create electronic transitions but it does contain enough energy to interact with a molecule causing vibrational and rotational changes. For example, the molecule can absorb the energy contained in the incident light and the result is a faster rotation or a more pronounced vibration. The possible rotations are around the axis of symmetry for a given molecule or either of the two perpendicular axis'. Vibrations can be in the form of a ¹bend or a ²stretch for each bond. Illustrated below are possible vibrational motions for a three atom molecule (all are in the plane unless explicitly stated):



(+ means out of screen and - is into screen)

The set of equations below accounts for only one absorption but experimental studies found that there were multiple peaks for each individual molecule. Quantum Mechanics describes the different absorption maxima as J^{th} level vibrational states that account for these other frequencies observed. There are $3N-5$ vibrational states for linear molecules and $3N-6$ vibrational states for non-linear molecules where N is the number of atoms. For more information, see [vibrational modes](#).

$$F = -ky$$

$$dE = -F dy$$

$$\int_0^E dE = \int_0^y ky dy$$

linear: $3N-5$ vib. states
non-linear: $3N-6$ vib. states

This equation describes the potential energy of the vibration

$$E = \frac{1}{2}ky^2$$

Because

$$F = ma$$

$$m \frac{d^2y}{dt^2} = -ky$$

This equation describes the periodic vibrational motion
 $y = A \cos(2\pi\nu_{\mu}t)$

Where

μ = the reduced mass

$$\frac{d^2y}{dt^2} = -4\pi^2\nu_\mu^2 A \cos(2\pi\nu_\mu t)$$

Therefore,

$$\nu_\mu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}$$

This is for the natural frequency of oscillation.

Instrument

The components of an IR machine are the IR source, beam splitter, monochromator, a transducer, an analog to digital converter and a digital machine to quantify the readout.¹ The IR light exits the source and becomes split into two beams, one to be directed to the sample the other to a reference. The intensity of the beam is measured by the intensity emitted divided by the intensity observed, also known as the Transmittance. All frequencies are measured in wavenumber, cm^{-1} . To make a sample with a liquid, the liquid is placed between two pure salt sheets of NaCl and for a solid it is pressure pressed with KBr to incorporate both into one sheet. The reason for using salt to suspend the molecule is because the salt structures form a lattice that is strongly ionically bonded and will not absorb IR light because it lacks the vibrational capability.³ The Background scan or reference tends to be air. *NaCl*

Below 1500 cm^{-1} the spectra have very high sensitivity and this region is known as the fingerprint region where C-C bond stretching and bending motions overlap, making it difficult to predict functional groups.⁵

For more specific bond stretch frequencies see [Characteristic Absorption Frequencies in IR Spectra](#)

Examples of Infrared Spectra

Example 1