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EFFECT OF THE OSCILLATING ELECTRIC FIELD DUE TO THE OSCILLATING ELECTRIC DIPOLE ON RAMAN LINES

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Raman Effect is the measurement of the intensity and wavelength of the inelastically scattered radiation that falls on a molecule. The electric field of the incident radiation polarizes the molecule on which it falls and this leads to the creation of an oscillating dipole. The incident polarized laser light is inelastically scattered by the molecular sample. The scattered light contains modified wavelengths called the Stokes and anti-Stokes lines or wavelengths. The oscillating electric dipole, created by the incident radiation, creates an oscillating electric field around it. Since the oscillating electric field of the incident radiation creates an oscillating electric dipole that create an oscillating electric field around it, it was surmised that this oscillating electric field can affect the frequency of vibration or oscillation of the oscillating electric dipole that produces it. This novel effect will change the frequency (frequencies) of the scattered radiation resulting in Stokes and anti-Stokes lines with modified frequencies. This theoretical research and its importance can be understood like this. For instance, if there are two cells or molecules, side by side, in which one is a healthy cell and the other is cancerous, or two different types of molecules are sitting side by side, this types of scattering should be able to distinguish one from the other since the Stokes and anti-Stokes lines from the two molecules will not be identical. Thus, the incident radiation of angular frequency ω_1 polarizes the charges of the molecule on which it falls and this leads to the creation of an oscillating dipole of frequency ω₂. The oscillating dipole creates an oscillating electric field that can create additional frequency of the oscillating dipole that created it, and let this be ω_D . Then the Raman lines can have frequencies $(\omega_1 + \omega_2 + \omega_D)$, $(\omega_1 + \omega_2 - \omega_D)$, $(\omega_1 - \omega_2 + \omega_D)$, and $(\omega_1 - \omega_2 - \omega_D)$. Depending on the relative magnitudes of ω_2 and ω_D , Raman lines will be designated as Stokes and Anti-Stokes lines. Due to the law of conservation of energy, ω_{DW} be less than ω_{D} since an oscillating dipole cannot create field of frequency more than its own frequency. Hence the frequencies $(\omega_1 - \omega_2 + \omega_D)$ and $(\omega_1 - \omega_2 - \omega_D)$ correspond to Stokes lines, and frequencies. $(\omega_1 + \omega_2 + \omega_D)$ and $(\omega_1 + \omega_2 - \omega_D)$ will correspond to Anti-Stokes lines. Calculations for Stokes and Anti-stokes lines have been done for some molecules, namely Ammonia compound (NH₃), Nitrousoxide compound (N₂O), Water (H₂O), Sulphur dioxide compound (SO₂), Ozone compound (O₃). Calculations have also been done for compounds containing carbon, such as Dichloromethane compound (CH₄Cl₂), Formic acid compound (CH₂O₂), Methanol compound (CH₄O), Benzene compound (C₆H₆), Propane compound (C₃H₈), and Carbonyl chloride compound (Cl₂CO). The theory developed predicts new phenomena of getting Stokes and anti-Stokes lines with modified wavelengths which have not been observed experimentally as of to-day.

KEYWORDS: electric dipole, Raman lines, Stokes lines, anti-Stokes lines, oscillating electric dipole

Inelastic scattering of light by a molecular sample was first predicted theoretically by Adolf Smekel [1] in 1923. The phenomenon was experimentally discovered in 1928 by an Indian Scientist C.V Raman [2,3]. He discovered the phenomena using filtered sunlight as a monochromatic source of photons, a colored filter as a monochromator, and a human eye as a detector. Originally Raman and Krishna observed the scattering of spectrally filtered sunlight from a liquid and observed that the scattered light contained very weak signals of light that had slightly different frequencies compared to the frequency of the incoming light. Some of the incident photons are elastically scattered (Rayleigh scattering), and it is found that hardly 1 in 10⁷ incident photons are elastically scattered. The number of inelastically scattered photons is much less. Quantum-mechanically, this process of scattering is interpreted as the shifted quantum states of the molecule. However, the intensity of the Raman signal is very low since hardly in 1 in 108 incident photons are inelastically scattered. The shifted quantum states lead to shifted frequencies in the scattering process, and these appear symmetrically around the frequency of the exciting radiation. This leads to the conclusion that the molecule may be either excited or de-excited during the scattering process. If the molecule is excited before the scattering event, it leads to Stokes scattering i.e., if ω_{laser} is the frequency of the incident light and ω_{s} is the frequency of the scattered light, then the Raman shift in frequency (Stokes lines) is $\Delta \omega = \omega_{laser} - \omega_s$ which is positive. However, when the molecule is de-excited, the Raman shift in the frequency will be such that $\omega_s > \omega_{laser}$, and these Raman lines are called anti-Stokes lines. Hence, the frequencies of the Raman lines depend on the states of excitation of the molecule on which the incident radiation falls.

Now it is well known that when light falls on a molecule, the molecule is polarized by the electric field of the incident radiation (also called the incident field). Both linear and nonlinear optical effects can be understood as resulting from the interaction of the electric field component of the incident electromagnetic radiation with the charged particles of the molecule or material. In general, an applied electric field moves positive charges in the direction of the electric field, and negative charges in the opposite direction. The electric field associated with the visible and near-infrared range of the electromagnetic spectrum oscillates at frequencies in the range of the 103 THz. These driving frequencies are quite large such that light particles, like electrons in the molecules or material follow the rapid oscillations of the driving field. This

is not the case for nuclei that are heavy particles. As a result of the driving fields, the bound electrons are slightly displaced from their equilibrium position. This process creates induced oscillating dipole that creates oscillating electric field. This oscillating electric field can affect the state of polarization of the molecule that created it, and also the quantum states of the molecule. It is this phenomenon that motivated us to study its effect on the frequencies of the resulting Stokes and anti-Stokes lines. It needs to be emphasized that the spectroscopic technique based on Raman scattering has been widely used in chemical analysis, study of biomolecules, crystals and powders, food industry, medical and environmental applications. The greatest advantage of this technique is that it requires very little or no sample preparation. The theory developed in this manuscript and the experimental techniques that may be developed in future could be very useful in medical science since the technique could be used to locate the disease in hidden parts of the body without destroying or affecting any internal structure or organs of the body [4].

We will now describe the basic ideas that will lead to the development of the theory suggested in this paper. It is well known that a dipole creates an electric field, say E_d , that polarizes the solid [5-7]. If all the molecules of the system are at one place, they all get polarized (i.e. each molecule acquires an induced dipole moment) and each causes an electric field at some point r_0 where the local field is calculated. An oscillating molecule under the action of an electric field (E_i) from the incident radiation will develop an oscillating dipole resulting in the creation of an oscillating electric field (E_L) . The magnitude of the molecular response is proportional to the sum of all the fields (E_i+E_L) acting at the same or some point r_0 , and the sum of these fields is called primary field. More explicitly we write the fields at the position r_0 at the time t as, $E_i(r_0, t)$ and $E_L(r_0, t)$, and the primary field say,

$$E_{p}(r_{0},t)=E_{i}(r_{0},t)+E_{L}(r_{0},t). \tag{1}$$

Now if ω_1 is the frequency of the incident radiation, ω_2 is the frequency of vibration of the induced of the molecule receiving the incident radiation (the frequency of the induced dipole is not to be confused with the natural frequency of vibration of the molecule), and ω_D is the frequency of the oscillating electric field created by the oscillating molecular dipole, then the frequencies of the Raman scattering or Raman lines or Raman scattered radiation can be,

$$\mathbf{\omega}_1 + \mathbf{\omega}_2 + \mathbf{\omega}_D,$$
 (2)

$$\mathbf{\omega}_1 + \mathbf{\omega}_2 - \mathbf{\omega}_D,$$
 (3)

$$\mathbf{\omega}_1 - \mathbf{\omega}_2 + \mathbf{\omega}_D,$$
 (4)

$$\omega_1$$
- ω_2 - ω_D . (5)

Depending on the relative magnitudes of ω_2 and ω_D with respect to ω_1 , we can get Stokes and anti-Stokes lines. If $\omega_2 > \omega_D$, then the following frequencies will correspond to anti-Stokes lines, i.e.

$$\mathbf{\omega}_1 + \mathbf{\omega}_2 + \mathbf{\omega}_D \text{ and } \mathbf{\omega}_1 + \mathbf{\omega}_2 - \mathbf{\omega}_D,$$
 (6)

whereas the following will correspond to Stokes lines

$$\omega_1$$
- ω_2 + ω_D and ω_1 - ω_2 - ω_D . (7)

Now ω_I is the frequency of the incident radiation and this will be known since the frequency of the selected incident light radiation for the experiment will be known. Then ω_2 is the frequency of oscillation of the induced dipole and this will also be known for a given molecule. Now to calculate ω_D , we have to first calculate the oscillating electric field (E_L) of the oscillating dipole of the molecule, and then calculate the energy due to this oscillating electric field. If this energy is denoted by U, then $U=\hbar\omega_D$ will give the value of ω_D .

Some of the important objectives of this research are as follows:

- (i) Since the incident radiation creates oscillating dipole, and the oscillating dipole creates oscillating electric field, it must therefore affect the oscillating dipole. This in turn leads us to ω_D that results in Stokes and anti-Stokes lines with new frequencies.
- (ii) Electromagnetic field emitted or scattered by molecules located in close proximity can be used in areas such as chemical and material science art restorations, military, plasmonics nanoparticles, the existence of cancerous and healthy cells, infections and hereditary diseases [8-15].
- (iii) It may motivate scientist to develop intense electric field lasers so that the value of ω_D can be increased such that the phenomena can be easily observed experimentally.

As usual there could be a larger or small gap between the proposed theory and the design of an experiment that can lead to the observation of the phenomena. For instance, Raman scattering was theoretically proposed in 1923, but discovered in 1928 [1,2]. The theory of simulated emission was proposed by Albert Einstein in 1917, but laser was discovered in 1960. Quite a few examples such, assuperconductivity, can be worth mentioning.

FORMULATION

We have to calculate the oscillating electric field (E_L) of a dipole (oscillating dipole) when the charge at its two ends is alternating with the angular frequency ω (ω =2 π f). Thus we have alternating charges ^+q and ^-q such that,

$$q = Q\cos\omega t,$$
 (8)

where Q – Is the maximum value of the charge on either sides.

Now to calculate the value of the oscillating electric field (\mathbf{E}_L) at the point of observation P, we have to know the value of the electric field at point P due to both charges, ${}^{\dagger}\mathbf{q}$ and ${}^{\dagger}\mathbf{q}$. Thus to know the value of E_L at P due to the charges, we must consider that the apparent value of the charge is not \mathbf{q} given as by Eqn. (8), but the value of \mathbf{q} at some earlier moment. This is the moment at which a disturbance would have had to be emitted by the charge, and travelling at the speed of light \mathbf{c} , to reach at the point P. The time of delay is $\frac{r_1}{c}$, and hence the apparent value of the charge will be

$$q_1 = Q\cos\omega\left(t - \frac{r_1}{c}\right),\tag{9}$$

where r_1 - distance between the center of the dipole and the point of observation P.

Similarly, for the charge q2, we write

$$q_2 = -Q\cos\omega\left(t - \frac{r_2}{c}\right). \tag{10}$$

It should be noted that the apparent charge is a function of its distance from the observer (point P), and this is clear from Eqn. (9) and Eqn. (10). Secondly, with the oscillating dipole, the amount of this time delay is different for the two charges since they are at different distances $(r_1 \neq r_2)$ from P(only when $\Theta = 90^0 = \frac{\pi}{2}$, that $r_1 = r_2$). Thus viewed in this way, the apparent total charge on the dipole is not zero $(q_1 \neq q_2)$ but fluctuates between positive and negative values. The apparent charge q_{app} can be written as,

$$q_{app} = q_1 + q_2 = Q \left[\cos \omega \left(t - \frac{r_1}{c} \right) - \cos \omega \left(t - \frac{r_2}{c} \right) \right]$$

= $-2Q \sin \omega \left(t - \frac{r}{c} \right) \sin \left(\frac{\omega l}{2c} \cos \theta \right),$ (11)

where it is assumed that $r \gg l$, and

$$r = \frac{1}{2}(r_1 + r_2)$$
 and $r_1 - r_2 \cong -l\cos\theta$, (12)

where l is the distance between the charges +q and -q.

We should note that when $\omega = 0$ (static dipole), $q_{app} = 0$, the field is localized and no oscillations. Now since ω is finite and the apparent value of the total charge is not zero, the field has a longer range, and falls off less rapidly with the distance. Assuming that the length of the dipole is very short compared to the wavelength, λ , of the disturbance it sends out, we can write,

$$\frac{l}{\lambda} = \frac{\omega l}{2\pi c} \ll 1 \qquad \left(\lambda = \frac{c}{f} = \frac{2\pi c}{\omega}\right). \tag{13}$$

Using Eqn. (13) in Eqn. (11), we can write $\sin \theta \cong \theta$ when θ is very small, and hence Eqn. (11) can be written as,

$$q_{app} \cong -\frac{\omega l}{c} Q \cos \theta \cdot \sin \omega \left(t - \frac{r}{c} \right).$$
 (14)

Here Ql is the maximum value of the dipole moment p_0 of the dipole, such that we can write,

$$p_0 = Ql, (15)$$

and

$$q_{app} = -\frac{\omega p_0}{c} \cos \theta \cdot \sin \omega \left(t - \frac{r}{c} \right). \tag{16}$$

We have now to evaluate the potential, v, which the dipole produces at the point P. If v_1 is the potential at P due to the upper charge, and v_2 is the potential at P due to the lower charge, then,

$$v = v_1 + v_2, (17)$$

where

$$v_1 = \frac{q_1}{4\pi\varepsilon_0 r_1},\tag{18}$$

$$v_2 = \frac{q_2}{4\pi\varepsilon_0 r_2}. (19)$$

Combining Eqns. (9), (10), (17), (18) and (19), we can write,

$$v = v_1 + v_2 = \frac{Q}{4\pi\varepsilon_0} \left[\frac{\cos\omega(t - \frac{r_1}{c})}{r_1} - \frac{\cos\omega(t - \frac{r_2}{c})}{r_2} \right]. \tag{20}$$

Assuming that the size of the dipole, l is very small compared to r_1 and r_2 then r_1 and r_2 may be almost equal to each other. Using the approximations, we get,

$$v = -\frac{\varrho l}{4\pi\varepsilon_0} \frac{\partial}{\partial z} \left[\frac{\cos\omega \left(t - \frac{r}{c}\right)}{r} \right]. \tag{21}$$

Eqn. (21) gives the basic formula for the potential due to the oscillating dipole. By putting $\omega = 0$, we get the potential for a stationary dipole. Eqn. (21) can be rewritten as,

$$v = -\frac{Ql}{4\pi\varepsilon_0} \frac{\partial}{\partial r} \left[\frac{\cos\omega(t - \frac{r}{c})}{r} \right] \frac{\partial r}{\partial z}.$$

$$= -\frac{Ql}{4\pi\varepsilon_0} \cdot \cos\theta \cdot \frac{\partial}{\partial r} \left[\frac{\cos\omega(t - \frac{r}{c})}{r} \right]$$

$$= \frac{Ql}{4\pi\varepsilon_0} \cos\theta \cdot \left[\frac{\cos\omega(t - \frac{r}{c})}{r^2} - \frac{\omega\sin\omega(t - \frac{r}{c})}{r} \right]. \tag{22}$$

Here in Eqn. (22), the first term refers to the static potential ($\omega = 0$), and the second term gives the electrostatic potential that would be produced by the apparent charge q_{app} given by Eqn. (16). In order to get the limiting form of v for large distances, r. It is evident that the second term in Eqn. (22) becomes quite large compared to the first term (since the second term has r in the denominator, and the first term has r^2 in the denominator). Thus the asymptotic value of v can be written as,

$$v \cong -\frac{\varrho l\omega}{4\pi\varepsilon_0 c}\cos\theta \cdot \frac{\sin\omega(t-\frac{r}{c})}{r}.$$
 (23)

From Eqn. (23) we can calculate the electric field strength E in polar coordinates r, θ , \emptyset . It can be shown that at large distance r, the components of E that are denoted by E_r (in the direction of increasing r), E_{θ} , (in the direction of increasing θ), and E_{\emptyset} (in the direction of increasing θ) have different values. In fact,

$$E_r \cong 0 \ and \ E_\emptyset = 0, \tag{24}$$

whereas,

$$E_{\theta} \cong \frac{Ql\omega^2}{4\pi\varepsilon_0 c^2} \sin\theta \frac{\cos\omega(t - \frac{r}{c})}{r}.$$
 (25)

Eqn. (25) shows that at large distances from the dipole the electric field $E \cong E_{\theta}$ becomes entirely transverse, at whatever direction relative to the dipole it is measured, and transversality is a necessary condition for the plane electromagnetic radiation. (At large distances from the source, any wave become a plane wave).

It is important to understand that Raman Effect is a result of inelastic interaction between light and matter. This interaction can in turn, generate linear and nonlinear optical phenomena, depending on the strength of the applied electric field and the nature of the sample on which light falls. For instance, the electric field intensities must be higher than typically 10^9 V/m to make the contributions of the induced dipole moment large enough to create a nonlinear effect in the medium [16]. Such high electric field intensities can be obtained by using giant- pulse lasers. In fact, linear scattering can be obtained when the frequency of the incident light (stream of photons) ω_0 is far away from the molecular electronic absorption frequency ω_1 such that $\omega_v \ll \omega_0 \ll \omega_1$, where ω_v is the vibrational frequency of the molecule. This is in line with the restriction of photon wavelength (energy) which lies in between the visible and near-visible regions and corresponds to vibrational and electronic molecular excitation energies. In this case, the photon transfers its energy $(\hbar\omega_0)$ to the whole molecule in order to displace the electron and produce an induced dipole moment. However, the electron remains bound since the large mass of the molecule does not allow such a transition. Hence, most of the incident light (photon) is transmitted without change of frequency and this type of scattering is called Rayleigh scattering, and is also known as elastic scattering.

It is necessary to understand that the origin of the Stokes and anti-Stokes scattering can be explained in terms of energy transfer between the incident light (photons) and the scattering system. When the molecule is initially excited to a level above the ground state, the scattered photon will gain energy and this scattering is termed as anti-Stokes scattering when the energy of the scattered radiation is $\hbar(\omega_0 + \omega_v)$. However, if the molecule is initially at the lowest level (the ground state), the scattered photon will lose energy and is called Stokes scattering whose energy is $\hbar(\omega_0 - \omega_v)$ [17].

The magnetic field associated with the radiation emitted by the oscillating dipole is, B, i.e.

$$B = \frac{Ql\omega^2}{4\pi\varepsilon_0 c^3} \sin\theta \cdot \frac{\cos\omega(t - \frac{r}{c})}{r}.$$
 (26)

Now E_{θ} and B are at right angles to \mathbf{r} , and at right angles to each other. The power radiated by the oscillating dipole will begiven by the Pointing vector 'S' [18] which is,

$$S = \frac{1}{\mu_0} (ExB),\tag{27}$$

where

$$\mu_0 = \frac{1}{\varepsilon_0 c^2}.\tag{28}$$

The average total power radiated is the surface integral of S over a sphere of radius r, and hence we get [6],

$$S = \frac{\mu_0 \omega^4 p_0^2}{12\pi c} \text{ where } p_0 = Ql$$

$$= \frac{\omega^4 p_0^2}{12\pi \epsilon_0 c^3}$$
(29)

$$=\frac{\omega^4 p_0^2}{12\pi\varepsilon_0 c^3} \tag{30}$$

If ω_D is the angular frequency ($\omega_D = 2\pi f_D$) associated with this field, then we can write,

$$S = \hbar \omega_D. \tag{31}$$

Between Eqns. (30) and (31), we get,

$$\omega_D = \frac{\omega^4 p_0^2}{12\pi\varepsilon_0 c^3 \hbar}.\tag{32}$$

Another method of calculating the energy, U, associated with the electric field E_{θ} will be to calculate the work done by the electric field E_{θ} in the displacement of the charge say Q, i.e.,

$$U = E_{\theta}. q. r \tag{33}$$

$$= \frac{Qql\omega^2 \sin \theta}{4\pi\varepsilon_0 c^2} \left[\cos \omega \left(t - \frac{r}{c}\right)\right] \tag{34}$$

Now

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} +, (35)$$

and for small x, we can approximate,

$$\cos x = \left(1 - \frac{x^2}{2!}\right),\tag{36}$$

and hence U becomes,

tables below:

$$U = \frac{Qql\omega^2 \sin \theta}{4\pi\varepsilon_0 c^2} - \frac{Qql\omega^2 \sin \theta}{4\pi\varepsilon_0 c^2} \cdot \omega^2 \left(t - \frac{r}{c}\right)^2. \tag{37}$$

Under initial conditions at just t = 0, the second term will have c^4 in the denominator, and this term will be very small compared to the first term that will have c² in the denominator. Thus Eqn. (37) gives U as,

$$U = \frac{Qql\omega^2 \sin\theta}{4\pi\varepsilon_0 c^2} \tag{38}$$

Generally, the observations are made perpendicular to the z-axis, $\theta = 90^{\circ}$, $\sin \theta = 1$, and hence,

$$U = \frac{Qql\omega^2}{4\pi\varepsilon_0 c^2}$$

$$= \frac{qp_0\omega^2}{4\pi\varepsilon_0 c^2} (p_0 = Ql)$$
(39)

$$=\frac{qp_0\omega^2}{4\pi\varepsilon_0c^2}(p_0=Ql)$$
 (40)

here Q=charge of one end of the electric dipole, q=electron charge.

Now if ω_D is the angular frequency associated with this energy, then,

$$U = \hbar \omega_D \text{ or } \omega_D = \frac{U}{\hbar} = \frac{p_0 \omega^2 q}{4\pi \varepsilon_0 c^2 \hbar}$$
 (41)

Now energy S given by Eqn. (30) is the energy radiated by the oscillating dipole, whereas the energy U given by Eqn. (40) is the energy fed into the oscillating dipole that was responsible for the creation of the oscillating electric field. It is this energy that can contribute to the Raman-shifted-frequencies or Raman scattering. Hence ω_D given by Eqn. (41) will affect the Stokes and anti-Stokes frequencies or lines.

RESULTS

Equations (41) have been used to determine angular frequency ω_D for some compounds whose Electric dipole moments and their angular frequency of vibration of the molecule were obtained from literature [19]. We considered krypton laser of the following wavelength (in nm):799.3, 752.5, 728.7, 676.4, 647.1, 632.8, 568.2, 530.9, 514.5, 488.0, 454.6, and 416.0, as incident radiation. The results of each compound considered are given in their respective

Ammonia compound (NH₃)

Electric dipole moment $(p_0) = 1.4718$ Debye

Angular frequency of vibration of the molecule (ω_2) = 6.2907×10¹⁴s⁻¹.

Angular frequency due to the electric dipole created by the vibrating molecule (ω_D) = 1.9405×10¹⁴s⁻¹

$\boldsymbol{\omega}_1 \times 10^{14} \mathrm{s}^{-1}$	$\omega_1 + \omega_2 + \omega_D$	$\omega_1 + \omega_2 - \omega_D$	ω_1 - ω_2 - ω_D	ω_1 - ω_2 + ω_D
45.3173	53.5485	49.6675	37.0861	40.9671
41.4694	49.7006	45.8196	33.2382	37.1192
38.6311	46.8623	42.9813	30.3999	34.2809
36.6414	44.8726	40.9916	28.4102	32.2912
35.5095	43.7407	39.8597	27.2783	31.1593
33.1785	41.4097	37.5287	24.9473	28.8283
29.7914	38.0226	34.1416	21.5602	25.4412
29.1331	37.3643	33.4833	20.9019	24.7829
27.8711	36.1023	32.2213	19.6399	23.5209
25.8707	34.1019	30.2209	17.6395	21.5205
25.0525	33.2837	29.4027	16.8213	20.7023
23.8564	32.0876	28.2066	15.6252	19.5062

Nitrous Oxide (N2O) compound

Electric dipole moment $(p_0) = 0.16083$ Debye

Angular frequency of vibration of the molecule (ω_2) = 4.1927×10¹⁴s⁻¹.

Angular frequency due to the electric dipole created by the vibrating molecule (ω_D) = 1.4217×10¹³s⁻¹.

$\omega_1 \times 10^{14} s^{-1}$	$\omega_1 + \omega_2 + \omega_D$	$\mathbf{\omega}_1 + \mathbf{\omega}_2 - \mathbf{\omega}_D$	ω_1 - ω_2 - ω_D	ω_1 - ω_2 + ω_D
45.3173	49.6522	49.3678	40.9824	41.2668
41.4694	45.8043	45.5199	37.1345	37.4189
38.6311	42.9660	42.6816	34.2962	34.5806
36.6414	40.9763	40.6919	32.3065	32.5909
35.5095	39.8444	39.5600	31.1746	31.4590
33.1785	37.5134	37.2290	28.8436	29.1280
29.7914	34.1263	33.8419	25.4565	25.7409
29.1331	33.4680	33.1836	24.7982	25.0826
27.8711	32.2060	31.9216	23.5362	23.8206
25.8707	30.2056	29.9212	21.5358	21.8202
25.0525	29.3874	29.3874	20.7176	21.0020
23.8564	28.1919	27.9069	19.2515	19.8059

Water (H₂O) compound

Electric dipole moment $(p_o) = 1.8546$ Debye

Angular frequency of vibration of the molecule (ω_2) = 6.8941×10¹⁴s⁻¹.

Angular frequency due to the electric dipole created by the vibrating molecule (ω_D) = 4.4327×10¹⁴s⁻¹.

$\omega_1 \times 10^{14} s^{-1}$	$\mathbf{\omega}_1 + \mathbf{\omega}_2 + \mathbf{\omega}_D$	$\mathbf{\omega}_1 + \mathbf{\omega}_2 - \mathbf{\omega}_D$	ω_1 - ω_2 - ω_D	ω_1 - ω_2 + ω_D
45.3173	56.6441	47.7787	33.9905	42.8559
41.4694	52.7962	43.9308	30.1426	39.0080
38.6311	49.9579	41.0925	27.3043	36.1697
36.6414	47.9682	39.1028	25.3146	34.1800
35.5095	46.8363	37.9709	24.1827	33.0481
33.1785	44.5053	35.6399	21.8517	30.7171
29.7914	41.1182	32.2528	18.4646	27.3300
29.1331	40.4599	31.5945	17.8063	26.6717
27.8711	39.1979	30.3325	16.5443	25.4097
25.8707	37.1975	28.3321	14.5439	23.4093
25.0525	36.3793	27.5139	13.7257	22.5911
23.8564	35.1832	26.3178	12.5296	21.3950

Sulphur dioxide (SO2) compound

Electric dipole moment $(p_o) = 1.63$ Debye

Angular frequency of vibration of the molecule (ω_2) = 2.1699×10¹⁴s⁻¹.

Angular frequency due to the electric dipole created by the vibrating molecule (ω_D) = 3.859×10¹³s⁻¹

$\omega_1 \times 10^{14} \text{s}^{-1}$	$\mathbf{\omega}_1 + \mathbf{\omega}_2 + \mathbf{\omega}_D$	$\mathbf{\omega}_1 + \mathbf{\omega}_2 - \mathbf{\omega}_D$	ω_1 - ω_2 - ω_D	$\mathbf{\omega}_1$ - $\mathbf{\omega}_2$ + $\mathbf{\omega}_D$
45.3173	47.8731	47.1013	42.7615	43.5333
41.4694	44.0252	43.2534	38.9136	39.6854
38.6311	41.1869	40.4151	36.0753	36.8471
36.6414	39.1972	38.4254	34.0856	34.8574
35.5095	38.0675	37.2935	32.9537	33.7255
33.1785	35.7343	34.9625	30.6227	31.3945
29.7914	32.3472	31.5754	27.2356	28.0074
29.1331	31.6889	30.9171	26.5773	27.3491
27.8711	30.4269	29.6551	25.3153	26.0871
25.8707	28.4265	27.6547	23.3149	24.0867
25.0525	27.6083	26.8365	22.4967	23.2685
23.8564	26.4122	25.6404	21.3006	22.0724

Ozone (O₃) compound

Electric dipole moment $(p_o) = 0.5337$ Debye

Angular frequency of vibration of the molecule (ω_2) = 2.0794×10¹⁴s⁻¹.

Angular frequency due to the electric dipole created by the vibrating molecule (ω_D) = 1.161×10¹³s⁻¹.

$\omega_1 \times 10^{14} \text{s}^{-1}$	$\omega_1 + \omega_2 + \omega_D$	$\omega_1 + \omega_2 - \omega_D$	ω_1 - ω_2 - ω_D	ω_1 - ω_2 + ω_D
45.3173	47.5128	47.2806	43.1218	43.3540
41.4694	43.6649	43.4327	39.2739	39.5061
38.6311	40.8266	405944	36.4356	36.6678
36.6414	38.8369	38.6047	34.4459	34.6781
35.5095	37.7045	37.4725	33.3140	33.5462
33.1785	35.3740	35.1415	30.9830	31.2152
29.7914	31.9869	31.7547	27.5959	27.8281
29.1331	31.3286	31.0961	26.9376	27.1698
27.8711	30.0666	29.8344	25.6756	25.6756
25.8707	28.0662	27.8340	23.6752	23.9074
25.0525	27.2480	27.0158	22.8570	23.0892
23.8564	26.0519	25.8197	21.6609	21.8931

Compounds with Carbon

Dichloromethane (CH₄CL₂) compound

Electric dipole moment $(p_o) = 1.60$ Debye

Angular frequency of vibration of the molecule (ω_2) = 5.6537×10¹⁴s⁻¹.

Angular frequency due to the electric dipole created by the vibrating molecule (ω_D) = 2.5719×10¹⁴s⁻¹.

$\omega_1 \times 10^{14} \text{s}^{-1}$	$\omega_1 + \omega_2 + \omega_D$	$\omega_1 + \omega_2 - \omega_D$	ω ₁ - ω ₂ - ω _D	ω_1 - ω_2 + ω_D
45.3173	53.5429	48.3991	37.0917	42.2355
41.4694	49.6950	44.5512	33.2438	38.3876
38.6311	46.8567	41.8129	30.4055	35.5493
36.6414	44.8670	39.7232	28.4158	33.5596
35.5095	43.7351	38.5913	27.2839	32.4277
33.1785	41.4041	36.2605	24.9529	30.0967
29.7914	38.0170	32.8732	21.5658	26.7096
29.1331	37.3587	32.2149	20.9075	26.0513
27.8711	36.0967	30.9529	19.6455	24.7893
25.8707	34.0963	28.9525	17.6451	22.7889
25.0525	33.2781	28.1343	16.8269	21.9707
23.8564	32.0820	26.9382	15.6308	20.7746

Formic acid (CH₂O₂) compound

Electric dipole moment $(p_o) = 1.425$ Debye

Angular frequency of vibration of the molecule (ω_2) = 4.9618×10¹⁴s⁻¹.

Angular frequency due to the electric dipole created by the vibrating molecule (ω_D) = 1.7642×10¹⁴s⁻¹.

$\omega_1 \times 10^{14} s^{-1}$	$\omega_1 + \omega_2 + \omega_D$	$\omega_1 + \omega_2 - \omega_D$	ω_1 - ω_2 - ω_D	ω_1 - ω_2 + ω_D
45.3173	52.0433	48.5149	38.5913	42.1197
41.4694	48.1954	44.6670	34.7434	38.2718
38.6311	45.3571	41.8287	31.9051	35.4335
36.6414	43.3674	39.8390	29.9154	33.4438
35.5095	42.2355	38.7071	28.7835	32.3119
33.1785	39.9045	36.3761	26.4525	29.9809
29.7914	36.5174	32.9890	23.0654	26.5938
29.1331	35.8591	32.3307	22.4071	25.9355
27.8711	35.5971	31.0687	21.1451	24.6735
25.8707	32.5967	29.0683	19.1447	22.6731
25.0525	31.7785	28.2501	18.3265	21.8549
23.8564	30.5824	27.0540	17.1304	20.6588

Methanol (CH₄O) compound

Electric dipole moment $(p_0) = 1.7$ Debye

Angular frequency of vibration of the molecule (ω_2) = 6.9394×10¹⁴s⁻¹.

Angular frequency due to the electric dipole created by the vibrating molecule (ω_D) = 4.1168×10¹⁴s⁻¹.

$\omega_1 \times 10^{14} s^{-1}$	$\omega_1 + \omega_2 + \omega_D$	$\omega_1 + \omega_2 - \omega_D$	ω_1 - ω_2 - ω_D	ω_1 - ω_2 + ω_D
45.3173	56.3735	48.1399	34.2611	42.4947
41.4694	52.5256	44.2920	30.4132	38.6468
38.6311	49.6873	41.4537	27.5785	35.8085
36.6414	37.6976	39.4640	25.5852	33.8188
35.5095	46.5657	38.3321	24.4533	32.6869
33.1785	44.2347	36.0011	22.1223	30.3559
29.7914	40.8476	32.6140	18.7352	26.9688
29.1331	40.1893	31.9557	18.0769	26.3105
27.8711	38.9273	30.6937	16.8149	25.0485
25.8707	36.9269	28.6933	14.8145	23.0481
25.0525	36.1087	27.8751	13.9963	22.2299
23.8564	34.9126	26.6790	12.8004	21.0338

Benzene (C₆H₆) compound

Electric dipole moment $(p_o) = 0.4236$ Debye

Angular frequency of vibration of the molecule (ω_2) = 4.3228×10¹⁴s⁻¹.

Angular frequency due to the electric dipole created by the vibrating molecule (ω_D) = 3.9806×10¹³s⁻¹.

$\omega_1 \times 10^{14} s^{-1}$	$\omega_1 + \omega_2 + \omega_D$	$\mathbf{\omega}_1 + \mathbf{\omega}_2 - \mathbf{\omega}_D$	ω_1 - ω_2 - ω_D	ω_1 - ω_2 + ω_D
45.3173	50.0382	49.2420	40.5964	41.3926
41.4694	46.1903	45.3941	36.7485	37.5447
38.6311	43.3520	42.5558	33.9102	34.7064
36.6414	41.3623	40.5661	31.9205	32.7167
35.5095	40.2304	39.4342	30.7886	31.5848
33.1785	37.8994	37.1032	28.4576	29.2538
29.7914	34.5123	33.7161	25.0705	25.8667
29.1331	33.8540	33.0578	24.4122	25.2084
27.8711	32.5920	31.7958	23.1502	23.9464
25.8707	30.5916	29.7954	21.1498	21.9460
25.0525	29.7734	28.9772	20.3316	21.1278
23.8564	28.5773	27.7811	19.1355	19.9317

Propane (C₃H₈) compound

Electric dipole moment $(p_0) = 0.084$ Debye

Angular frequency of vibration of the molecule (ω_2) = 5.6065×10¹⁴s⁻¹.

Angular frequency due to the electric dipole created by the vibrating molecule (ω_D) = 1.3278×10¹³s⁻¹.

$\omega_1 \times 10^{14} \text{s}^{-1}$	$\mathbf{\omega}_1 + \mathbf{\omega}_2 + \mathbf{\omega}_D$	$\omega_1 + \omega_2 - \omega_D$	ω_1 - ω_2 - ω_D	ω_1 - ω_2 + ω_D
45.3173	51.0566	50.7910	39.5780	39.8436
41.4694	47.2087	46.9431	35.7301	35.9957
38.6311	44.3704	44.1048	32.8918	33.1574
36.6414	42.3807	42.1151	30.9021	31.1677
35.5095	41.2488	40.9832	29.7702	30.0358
33.1785	39.9178	38.6522	27.4392	27.7048
29.7914	35.5307	35.2651	24.0521	24.3177
29.1331	34.8724	34.6068	23.3938	23.6594
27.8711	33.6104	33.3448	22.1318	22.3974
25.8707	31.6100	31.3444	20.1314	20.3970
25.0525	30.7918	30.5262	19.3132	19.5788
23.8564	29.5957	29.3301	18.1171	18.3827

Carbonyl chloride (Cl2CO) compound

Electric dipole moment $(p_0) = 1.17$ Debye.

Angular frequency of vibration of the molecule (ω_2) = 1.0689×10¹⁴s⁻¹.

Angular frequency due to the electric dipole created by the vibrating molecule (ω_D) = 6.72×10¹²s⁻¹.

$\omega_1 \times 10^{14} \text{s}^{-1}$	$\omega_1 + \omega_2 + \omega_D$	$\omega_1 + \omega_2 - \omega_D$	ω_1 - ω_2 - ω_D	ω_1 - ω_2 + ω_D
45.3173	46.4534	46.3190	44.1812	44.3156
41.4694	42.6055	42.4711	40.3333	40.4677
38.6311	39.7672	39.6328	37.4950	37.6294
36.6414	37.7775	37.6431	35.5053	35.6397
35.5095	36.6456	36.5112	34.3734	34.5078
33.1785	34.3146	34.1802	32.0424	32.1768
29.7914	30.9275	30.7931	28.6553	28.7897
29.1331	30.2692	30.1348	27.9970	28.1314
27.8711	29.0072	28.8728	26.7350	26.8694
25.8707	27.0068	26.8724	24.7346	24.8690
25.0525	26.1886	26.0542	23.9164	24.0508
23.8564	24.9925	24.8581	22.7203	22.8547

DISCUSSION AND SUMMARY

There are a number of important reasons as to why the development of Raman spectroscopy was very slow. An important reason is that the Raman Effect is very weak [20]. Hardly one part in a million of the total intensity of the incident light is elastically scattered (Rayleigh scattering), whereas for Raman scattering this value is one part in 10⁸ of the incident light intensity [21]. This is also the most important reason that the discovery of Raman Effect was delayed. Even the discovery of laser was delayed up to 1960, but once a large number of lasers with powerful beams were discovered, new laser techniques stimulated the field of molecular spectroscopy and Raman spectroscopy.

Raman Effect arises when a photon is incident on a molecule, and it interacts with the dipole created by the electric field of the incident light radiation. In fact, an oscillating dipole is created. Now an oscillating dipole creates an oscillating electric field, and in this manuscript it is assumed that the oscillating electric field, created by the oscillating dipole can affect the frequency scattered due to the Raman Effect. The modification in the frequency of the Stokes and anti-Stokes lines due to this effect is calculated and is denoted as ω_D . The values of ω_D for different molecules have been calculated. These values are different for different molecules and are smaller than ω_1 and ω_2 by a factor of roughly 10. We emphatically believe that it should be possible to measure the value of ω_D by an appropriate experimental design and by using an intense electric field laser. One method could be that two laser beams are used. First a Q-switched laser beam (pulse of a beam) is projected on the molecule and then a continuous wave (CW) laser beam be projected on the same molecules. This process of getting Stokes and anti-Stokes lines may help in getting a specific value for ω_D for different molecules. This process can be called double beam Raman scattering. It is not easy to surmise how soon the exact value of ω_D can be measured since the gap between theoretical prediction and experimental observation has beengenerally large. Moreover, an intense electric field laser can lead to larger ω_D values that can be measured. Intense electric field

can affect ω_D , but larger number of photons in the laser beam will affect the intensity of Raman lines. Typical electric field intensities of order of 10^{10} V/m or more may be required to obtain values of ω_D that can be measured.

Raman spectroscopy provides a unique biochemical study capable of identifying and characterizing the structure of molecules, tissues, and cells. In identifying cervical cancer, it is established that it is a promising biochemical tool due to its ability to detect pre-malignancy and early malignancy stages [11-13, 22-25]. Raman lines differ between normal and malignant biopsy samples. In our case it is the value of ω_D that will differ between normal and malignant biopsy samples.

A greater body of experimental evidence may be needed in future to establish the validity of the theory developed in this manuscript. However, the fact remains that the type of Raman scattering proposed in this manuscript can be observed experimentally, and it can become a promising biomedical tool, especially by obtaining Raman lines after radiotherapy cycles and so on.

The concept in this manuscript is that the molecule may be excited not only by the incident laser radiation but also by the oscillating electric field created by the oscillating dipole. It is quite possible that our study can be used in the study of Four-Wave mixing microscopy of nanostructures [26], and Surface-Enhanced Raman Spectroscopy (SERS), and Coherent Raman Spectroscopy (CARS) [27-30,]. We are not competent to say how the experiments may be designed to observe these phenomena.

We must point out that we have not been able to find out any theoretical and or experimental observations on these lines in literature. From the above results, it shows that the theory developed predicts new phenomena of getting Stokes and anti-Stokes lines with modified wavelengths. It is proposed that such a phenomenon may be observed experimentally by using intense electric field laser.

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ВПЛИВ ОСЦИЛЮЮЧОГО ЕЛЕКТРИЧНОГО ПОЛЯ ЧЕРЕЗ ОСЦИЛЛЯЦІЇ ЕЛЕКТРИЧНОГО ДИПОЛЯ НА РАМАНІВСЬКІ ЛІНІЇ Ханна М. Капіл¹, Мурей К. Гілберт²

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Ефект Рамана полягає у вимірюванні інтенсивності та довжини хвиль непружно розсіяного випромінювання, яке падає на молекулу. Електричне поле випромінювання поляризує молекулу, на яку вона падає, і це призводить до створення коливань диполя. Поляризоване лазерне світло, що падає, непружно розсіюється молекулярним зразком. Розсіяне світло містить змінені довжини хвиль, які називаються Стоксівськими та анти-Стоксівськими довжинами хвиль. Електричний диполь, що коливається внаслідок падаючого випромінювання, створює навколо себе коливальне електричне поле. Оскільки коливальне електричне поле падаючого випромінювання створює коливальний електричний диполь, який створює навколо нього коливальне електричне поле, то вважається, що це коливальне електричне поле може впливати на частоту коливань або коливання електричного диполя, який його виробляє. Цей новий ефект змінить частоту (частоти) розсіяного випромінювання, що призведе до появи ліній Стокса та анти-Стокса зі зміненими частотами. Це теоретичне дослідження та його значення можна пояснити наступним чином. Наприклад, якщо є дві клітини або молекули поруч, у яких одна є здоровою клітиною, а інша – раковою, або два різних типів молекул що знаходяться поряд, цей тип розсіювання повинен бути в змозі розрізнити одну ситуацію від іншої, оскільки лінії Стокса і анти-Стокса від двох молекул не будуть ідентичними. Таким чином падаюче випромінювання кутової частоти $\omega 1$ поляризує молекулу, на яку вона падає, і це призводить до створення коливального диполя частоти ω 2. Коливальний диполь створює коливальне електричне поле, яке може створити додаткову частоту коливального диполя, який його створив, і нехай це буде ωD . Тоді лінії Рамана можуть мати частоти ($\omega 1+\omega 2+\omega D$), $(\omega 1 + \omega 2 - \omega D)$, $(\omega 1 - \omega 2 + \omega D)$ та $(\omega 1 - \omega 2 - \omega D)$. Залежно від відносних величин $\omega 2$ і ωD , лінії Рамана будуть позначатися як лінії Стокса і анти-Стокса. Через закон збереження енергії фD буде менше ніж ф2, оскільки коливальний диполь не може створити поле частоти більше своєї власної частоти. Отже, частоти ($\omega 1$ - $\omega 2$ + ωD) і ($\omega 1$ - $\omega 2$ - ωD) відповідають лініям Стокса і частотам. $(\omega 1 + \omega 2 + \omega D)$ і $(\omega 1 + \omega 2 - \omega D)$ будуть відповідати лініям анти-Стокса. Розрахунки ліній Стокса та анти-Стокса були зроблені для деяких молекул: аміаку (NH₃), оксиду азоту (N₂O), води (H₂O), діоксиду сірки (SO₂), (O₃). Розрахунки також були проведені для сполук, що містять вуглець, таких як дихлорметан (CH₄Cl₂), мурашиної кислоти (CH₂O₂), метанолу (CH₄O), бензолу (С₆Н₆), пропану (С₃Н₈) та карбонілхлориду (СІ₂СО). Розроблена теорія передбачає нові явища для отримання ліній Стокса та анти-Стокса зі зміненою довжиною хвилі, які не спостерігалися експериментально на сьогоднішній день.

КЛЮЧОВІ СЛОВА: електричний диполь, лінії Рамана, лінії Стокса, анти-Стокса, коливальний електричний диполь

ВЛИЯНИЕ ОСЦИЛЛИРУЮЩЕГО ЭЛЕКТРИЧЕСКОГО ПОЛЯ ЧЕРЕЗ ОСЦИЛЛЯЦИИ ЭЛЕКТРИЧЕСКОГО ДИПОЛЯ НА РАМАНОВСКИЕ ЛИНИИ Xанна M. Kanuл I , Mypeŭ K. Γ илбер m^{2}

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Эффект Рамана состоит в измерении интенсивности и длины волн неупруго рассеянного излучения, которое падает на молекулу. Электрическое поле излучения поляризует молекулу, на которую она падает, и это приводит к созданию колебаний диполя. Поляризованный лазерный свет, падающий не упруго рассеивается молекулярным образцу. Рассеянный свет содержит изменены длины волн, которые называются Стоксовскими и анти-Стоксовскими длинами волн. Электрический диполь, который колеблется вследствие падающего излучения, создает вокруг себя колебательное электрическое поле. Поскольку колебательное электрическое поле падающего излучения создает колебательный электрический диполь, который создает вокруг него колебательное электрическое поле, то считается, что это колебательное электрическое поле может влиять на частоту колебаний или колебания электрического диполя, который его производит. Этот новый эффект изменит частоту (частоты) рассеянного излучения, что приведет к появлению линий Стокса и анти-Стокса с измененными частотами. Это теоретическое исследование и его значение можно объяснить следующим образом. Например, если есть две клетки или молекулы рядом, в которых одна является здоровой клеткой, а другая - раковой или два различных типов молекул, находящихся рядом, этот тип рассеяния должен быть в состоянии различить одну ситуацию от другой, поскольку линии Стокса и анти-Стокса от двух молекул не будут идентичными. Таким образом падающее излучение угловой частоты ω1 поляризует молекулу, на которую она падает, и это приводит к созданию колебательного диполя частоты $\omega 2$. Колебательный диполь создает колебательное электрическое поле, которое может создать дополнительную частоту колебательного диполя, который его создал, и пусть это будет ωD . Тогда линии Рамана могут иметь частоты ($\omega 1+\omega 2+\omega D$), ($\omega 1+\omega 2-\omega D$), ($\omega 1-\omega 2+\omega D$) и (ω 1- ω 2- ω D). В зависимости от относительных величин ω 2 и ω D, линии Рамана будут обозначаться как линии Стокса и анти-Стокса. Через закон сохранения энергии ωD будет меньше чем ω2, поскольку колебательный диполь не может создать поле частоты больше своей собственной частоты. Итак, частоты ($\omega 1$ - $\omega 2$ + ωD) и ($\omega 1$ - $\omega 2$ - ωD) соответствуют линиям Стокса и частотам. $(\omega 1 + \omega 2 + \omega D)$ и $(\omega 1 + \omega 2 - \omega D)$ будут соответствовать линиям анти-Стокса. Расчеты линий Стокса и анти-Стокса были сделаны для некоторых молекул: аммиака (NH3), оксида азота (N2O), воды (H2O), диоксида серы (SO2), озона (O3). Расчеты также были проведены для соединений, содержащих углерод, таких как дихлорметан (CH₂Cl₂), муравьиная кислота (CH₂O₂), метанола соединение (CH4O), бензола (C₆H₆), пропана (C₃H₈) и карбонилхлорида (Cl₂CO). Разработанная теория предполагает новые явления для получения линий Стокса и анти-Стокса с измененной длиной волны, что не наблюдались экспериментально на сегодняшний день.

КЛЮЧЕВЫЕ СЛОВА: электрический диполь, линии Рамана, линии Стокса, анти-Стокса, колебательный электрический липоль