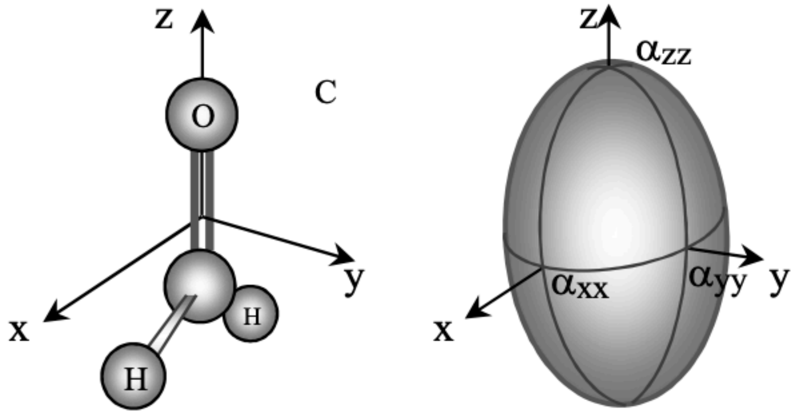
Raman Spectroscopy

Raman spectroscopy is an alternative way to get information about the **infrared transitions** within a molecule. In order for a vibrational transition to be Raman active, the molecule must undergo a change in polarizability during the vibration.

Polarizability refers to the ease of distorting electrons from their original position.

The polarizability of a molecule decreases with **increasing electron density, increasing bond strength**, and **decreasing bond length**.

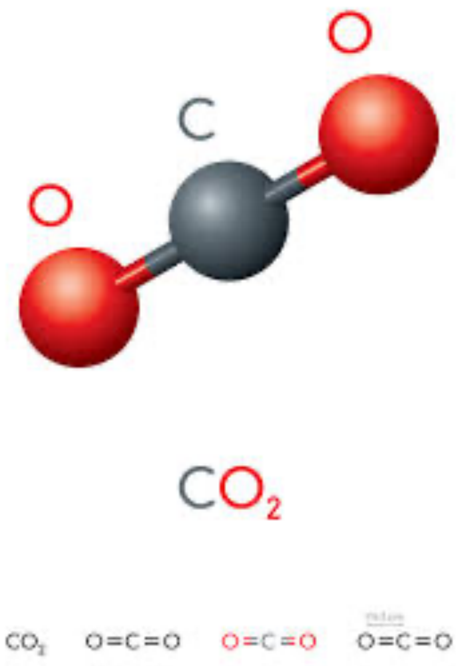


Is carbon dioxide IR inactive?

Incidentally, Carbon di-oxide is not only IR active, but a greenhouse gas because of the IR absorption in the atmosphere.

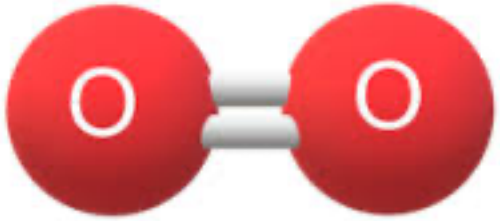
Carbon di-oxide doesn't have a static dipole,

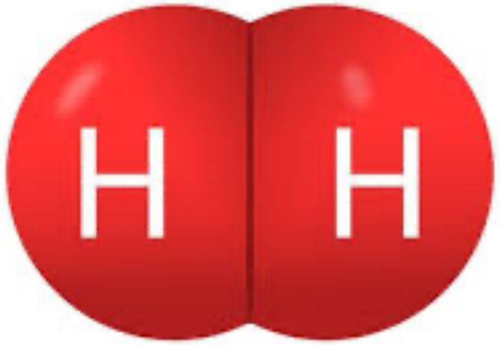
it can't be IR active

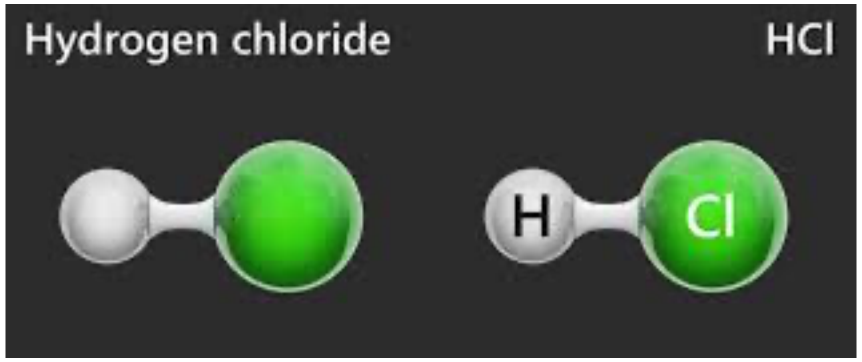


IR activity is the result of dynamic dipoles - meaning the dipole changes with some type of deformation motion; in the case of Carbon di-oxide this occurs with bending motion and asymmetric stretching, not static dipoles.

Types of Molecules and Rotational Raman Spectra







(i) Linear Molecules

In case of linear molecules, $I_B = I_C$ and $I_A \cong 0$. All such molecules like H_2, O_2, CO_2, HCl etc. exhibit rotational Raman spectra because their end-over-end rotations produce change in polarizability. However, rotation about the bond axis produces no change in polarizability.

(ii) Symmetric Top Molecules

In symmetric top molecules, $I_B = I_C$; $I_A \neq 0$. All such molecules like CH_3F and $CHCl_3$, exhibit rotational Raman spectra because rotation about the top axis (e.g. C—F bond axis in case of CH_3F) produces no change in the polarizability but end-over-end rotations produce such a change.

Types of Molecules and Rotational Raman Spectra

(iii) Spherical Top Molecules

Molecules like CH_4, CCl_4 etc. are spherical top. These have all the three moments of inertia identical

$$I_A = I_B = I_C$$

Owing to their symmetry, rotation alone can produce no change in the polarizability and hence no rotational Raman spectrum is observable.

(iv) Asymmetric Top Molecules

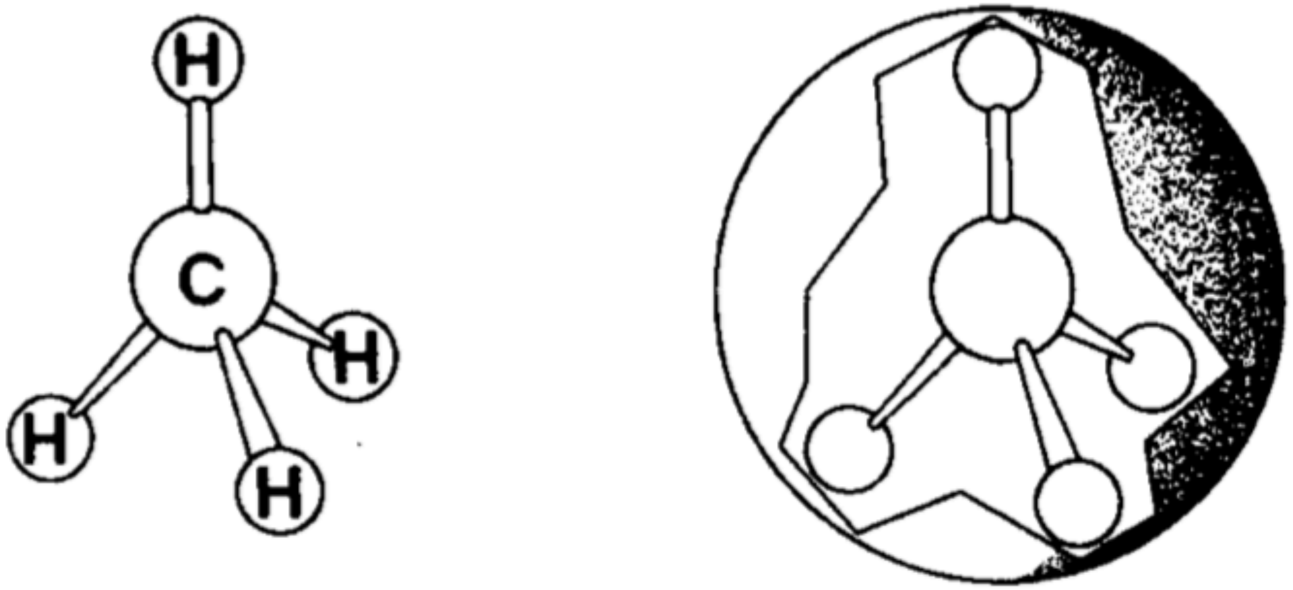
Majority of substances belong to this class of molecules. These have all the three moments of inertia different

$$I_A \neq I_B \neq I_C$$

Simple examples are water and vinyl chloride. All such molecules exhibit rotational Raman spectra. However, their Raman spectra are complicated because all rotations of these molecules are Raman active, i.e. they produce change in the polarizability.

Spherical Top Molecule

The tetrahedral molecule, methane



Polarizability ellipsoid is spherical. During the vibration known as the **symmetric stretch all four C-H distances** increase and diminish in phase so that the polarizability ellipsoid contracts and expands but *remains spherical*.

For this reason the motion is often referred to as the 'breathing frequency'; it is plainly **Raman active**.

In contrast, methane is not infrared active because it does not experience a change in permanent dipole whilst vibrating.

Consider the molecular vibrations of carbon dioxide and determine whether or not they are Raman active.

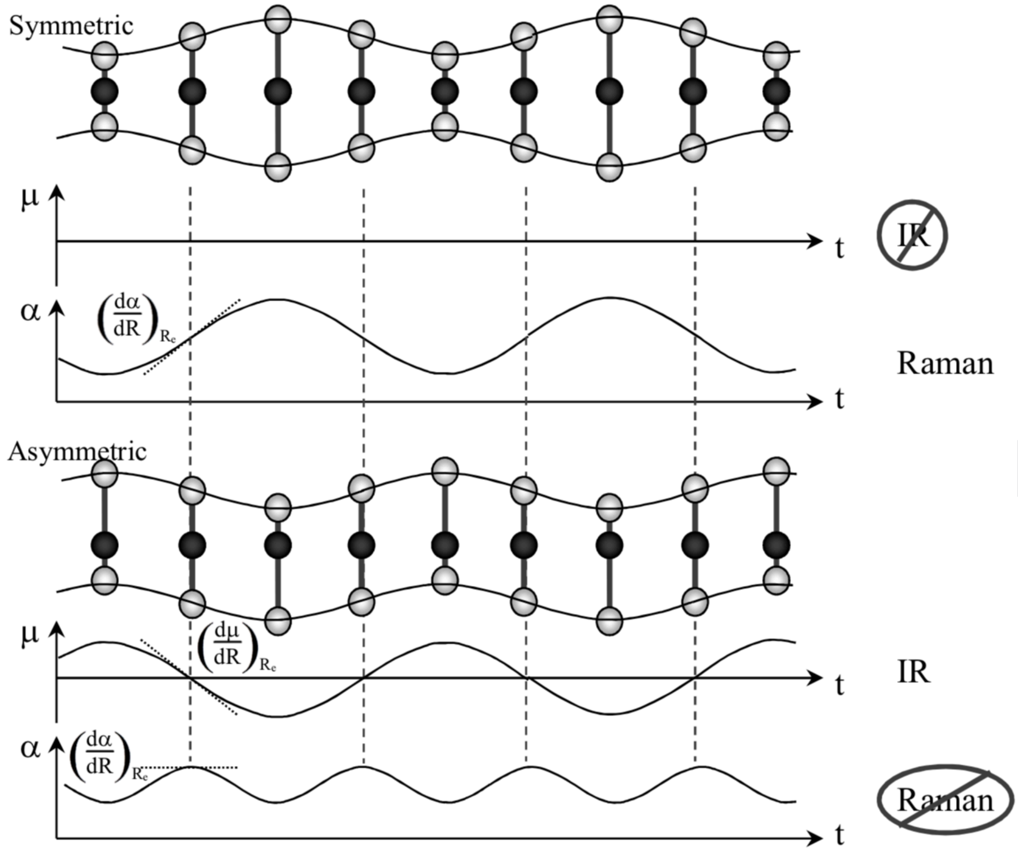
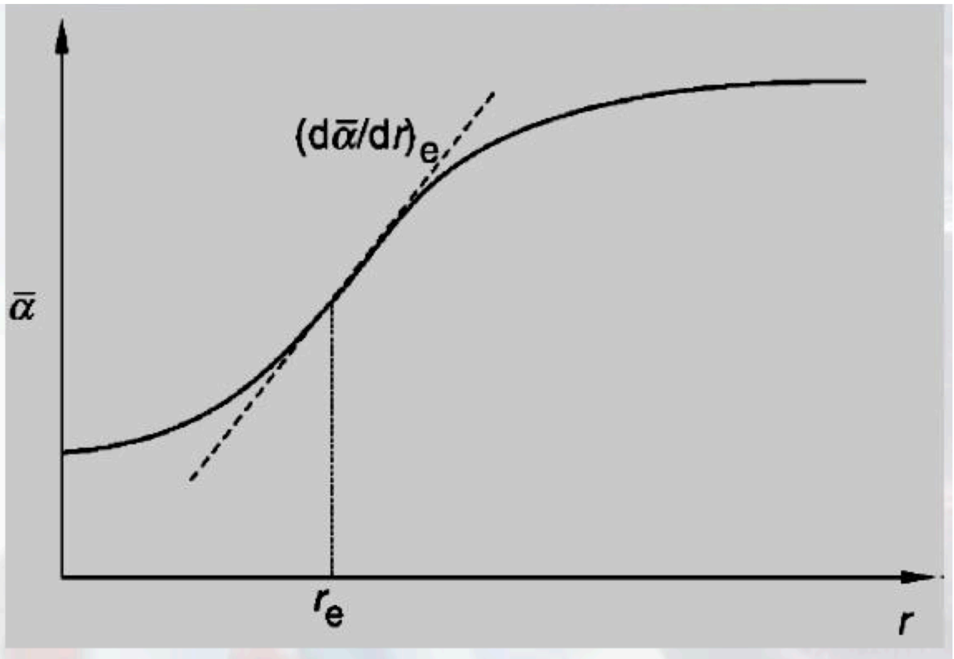


Figure 6: Symmetric and asymmetric stretch of CO_2. The equilibrium positions are at the dotted vertical line. The symmetric stretch gives no dipole moment; the symmetric stretch is infrared inactive and Raman active. The derivative of the polarizability for the asymmetric stretch of CO_2 vanishes; the asymmetric stretch is infrared active and Raman inactive.[8]



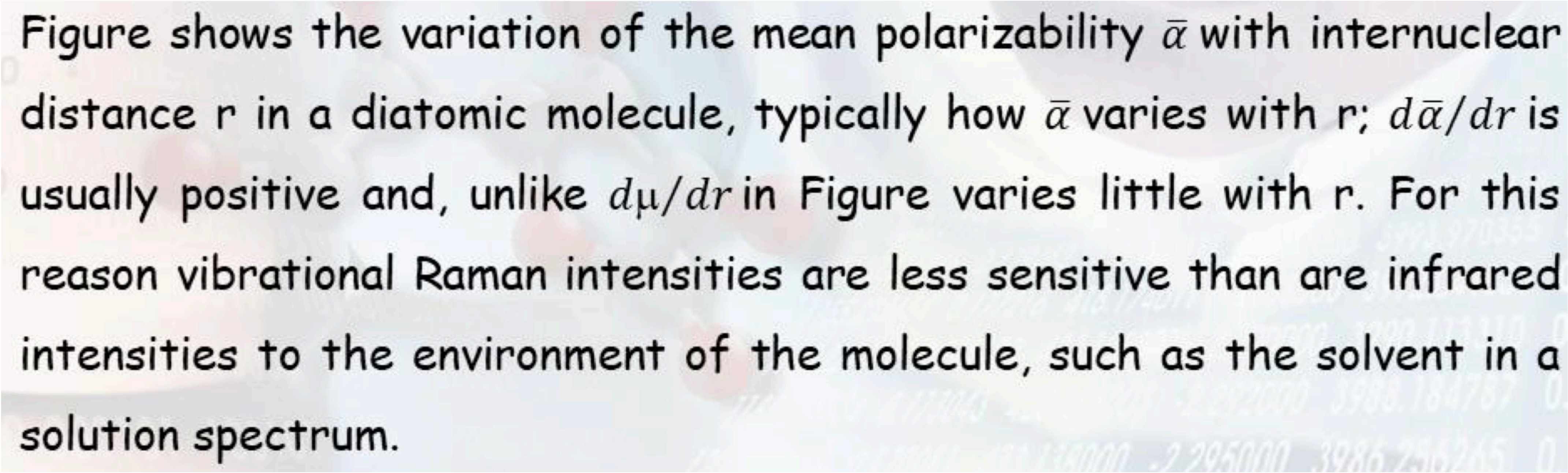
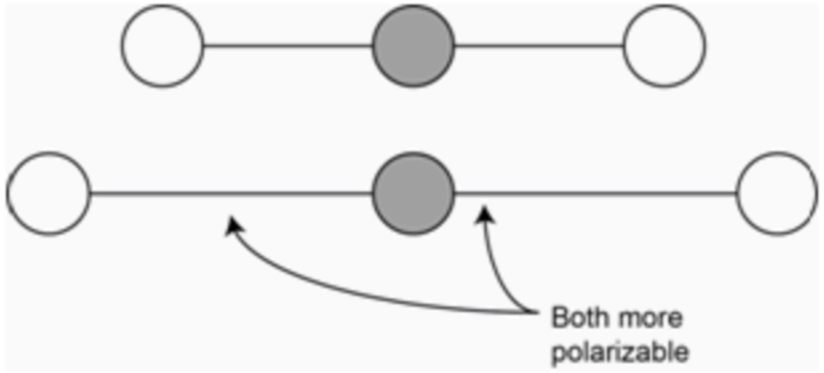
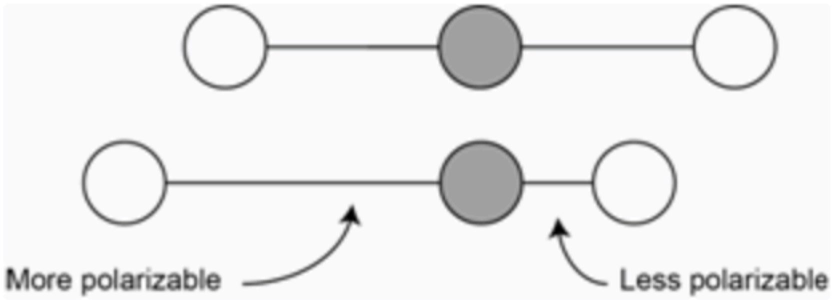
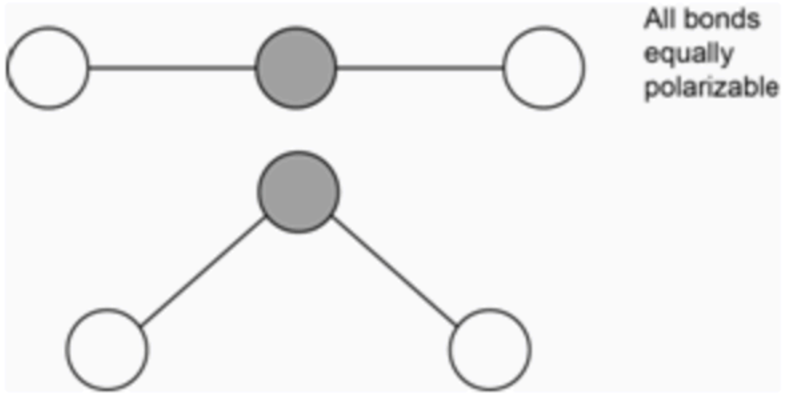


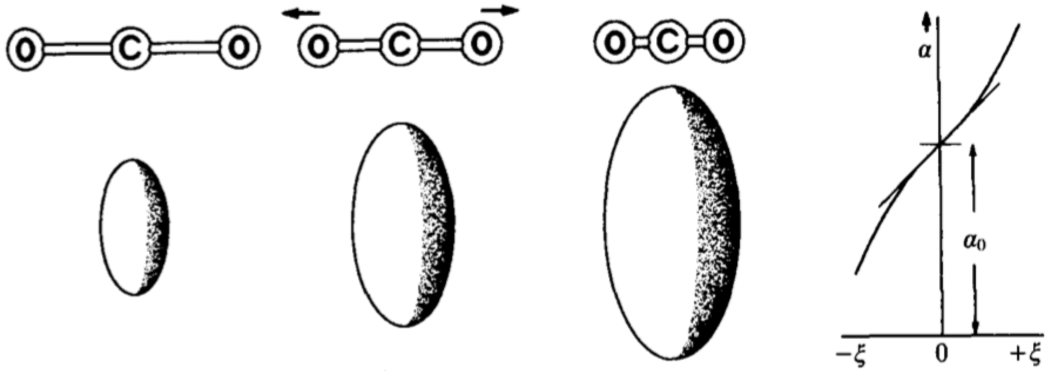
Figure shows the variation of the mean polarizability $\bar{\alpha}$ with internuclear distance r in a diatomic molecule, typically how $\bar{\alpha}$ varies with r; $d\bar{\alpha}/dr$ is usually positive and, unlike $d\mu/dr$ in Figure varies little with r. For this reason vibrational Raman intensities are less sensitive than are infrared intensities to the environment of the molecule, such as the solvent in a solution spectrum.

Consider the molecular vibrations of carbon dioxide and determine whether or not they are Raman active.

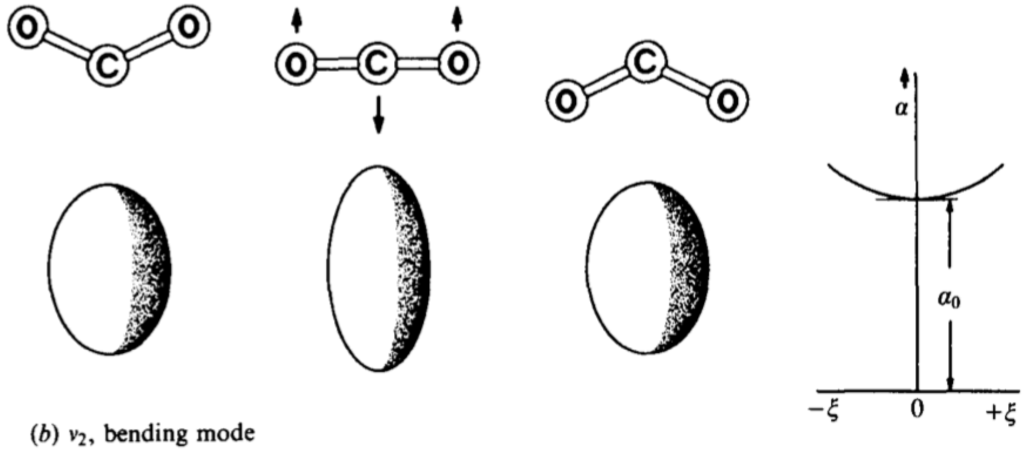




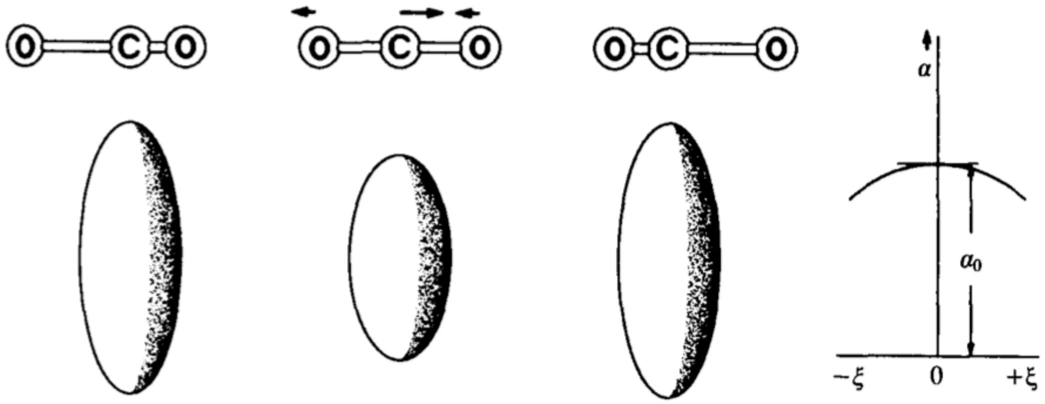




(a) ν_1, symmetric stretching mode



(b) ν_2, bending mode



(c) ν_3, asymmetric stretching mode

Figure 4.7 The changes in the polarizability ellipsoid of carbon dioxide during its vibrations, and a graph showing the variation of the polarizability, α, with the displacement coordinate, ξ, during each vibration.

Mutual exclusion rule

Rule of mutual exclusion. If a molecule has a *centre of symmetry* then Raman active vibrations are infra-red inactive, and vice versa. If there is no centre of symmetry then some (but not necessarily all) vibrations may be both Raman and infra-red active.

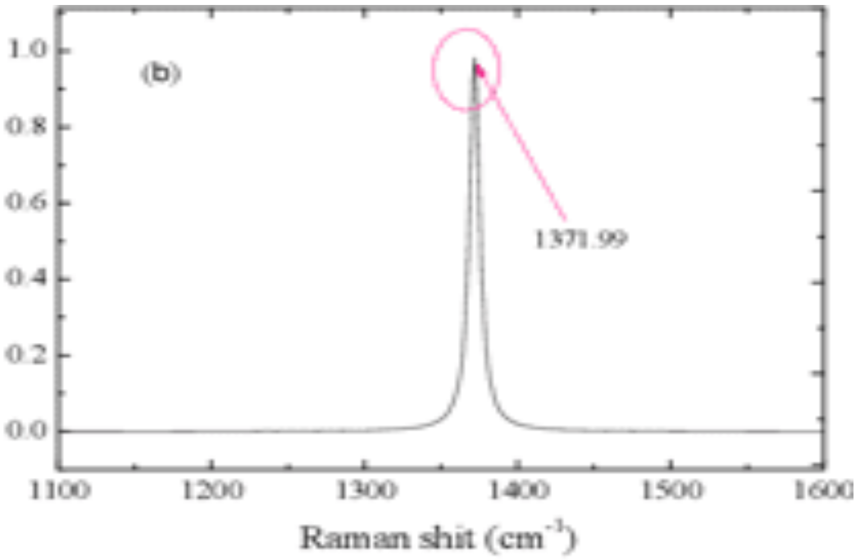
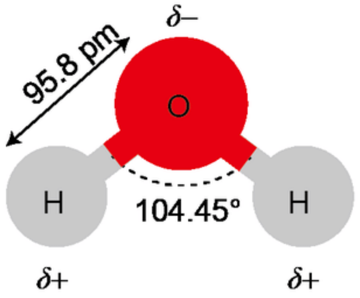
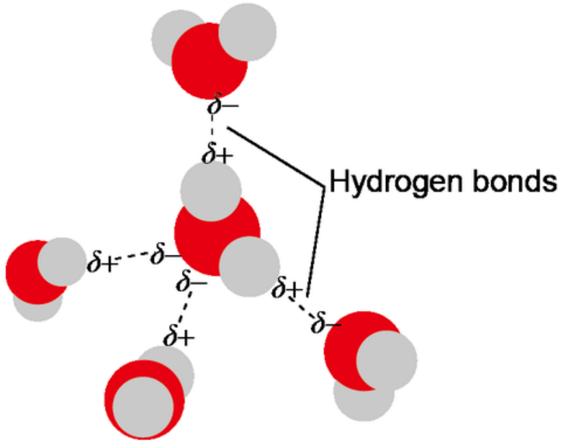


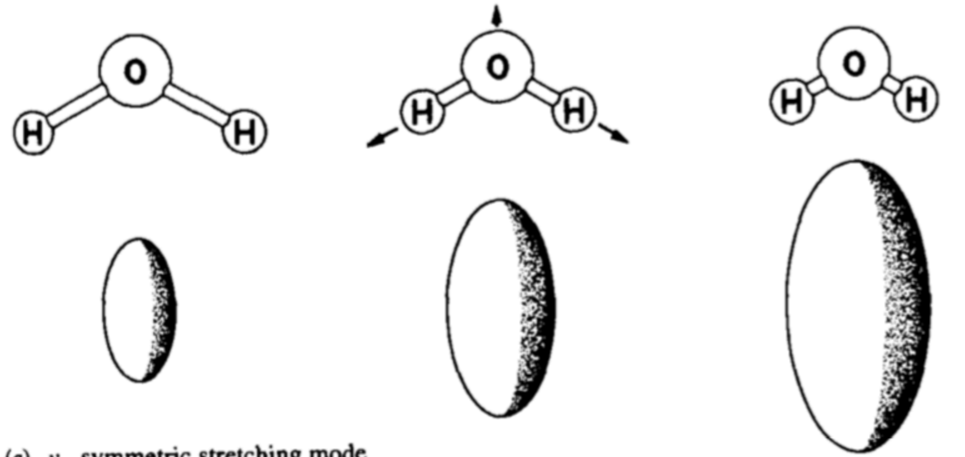
Table 4.1 Raman and infra-red activities of carbon dioxide

Mode of vibration of CO_2	Raman	Infra-red
ν_1 : symmetric stretch	Active	Inactive
ν_2 : bend	Inactive	Active
ν_3 : asymmetric stretch	Inactive	Active

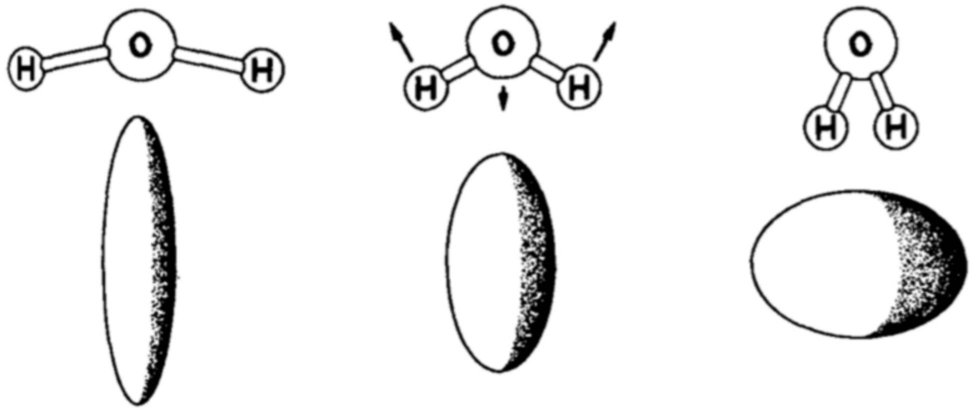
Assymetric top molecule



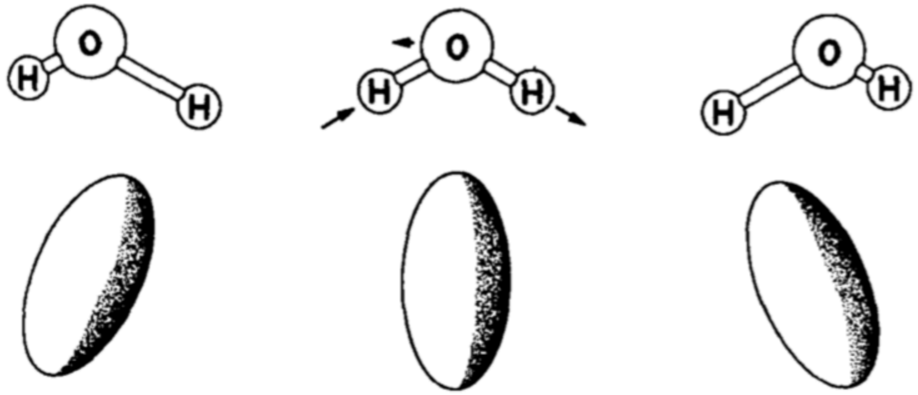




(a) ν_1, symmetric stretching mode



(b) ν_2, bending mode



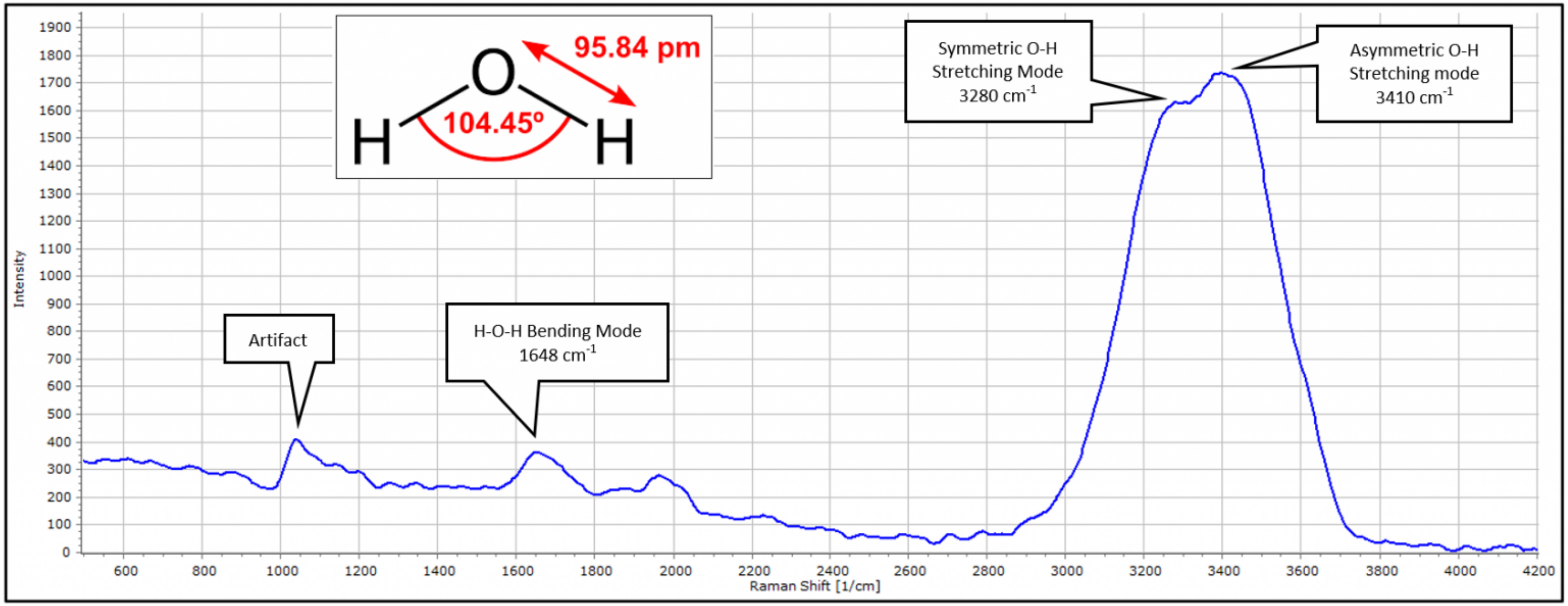
(c) ν_3, asymmetric stretching mode

Figure 4.6 The change in size, shape, or direction of the polarizability ellipsoid of the water molecule during each of its three vibrational modes. The centre column shows the equilibrium position of the molecule, while to right and left are the (exaggerated) extremes of each vibration.

$$\left(\frac{d\alpha}{dQ}\right)_e \neq 0$$

Since, **all three vibrations** of H_2O involve obvious changes in at least one aspect (size, shape or direction) of the polarizability ellipsoid, and all are **Raman active.**

Assymetric Top Molecule



Ref: https://physicsopenlab.org/2022/01/08/water-molecule-vibrations-with-raman-spectroscopy/

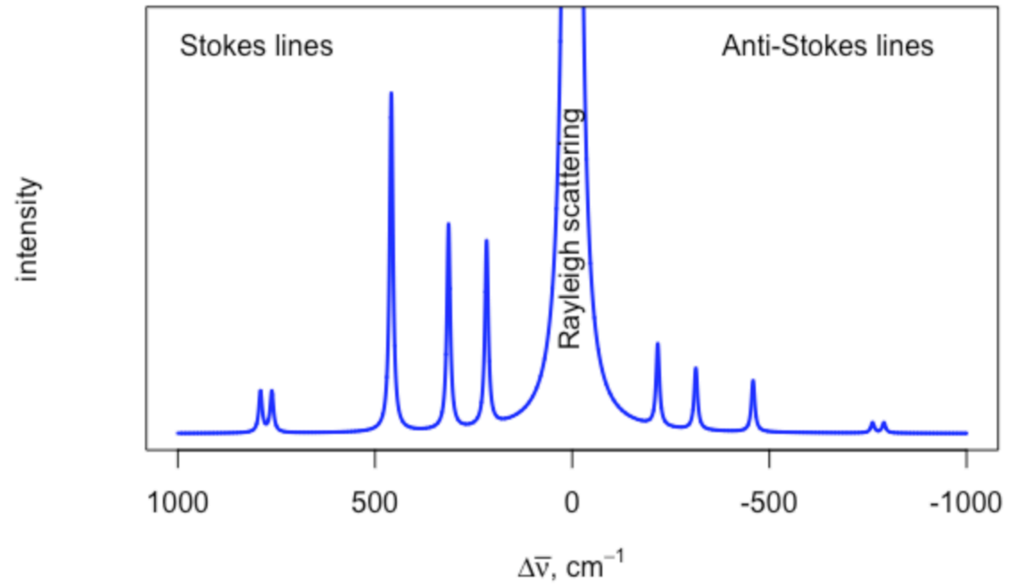
Symmetric vibration give rise to intense Raman lines; non-symmetric ones are usually weak and sometimes unobservable.

Important Features of Raman spectra of Carbon Tetrachloride (CCl_4)

First, Rayleigh scattering produces an intense peak at frequency of 0. Although the peak is intense, it carries no useful information as the absolute energy is just that for the source.

Second, Raman scattering has two components—Stokes lines and the anti-Stokes lines—that have identical absolute shifts relative to the line for Rayleigh scattering, but that have different signs

Figure 18.1.1: The Raman spectrum for carbon tetrachloride, CCl_4, showing the intense peak for Rayleigh scattering at $\Delta\bar{\nu} = 0$ and five lines each for Stokes and anti-Stokes scattering with $\Delta\bar{\nu} = \pm 217.0\ \text{cm}^{-1}$, $\Delta\bar{\nu} = \pm 313.5\ \text{cm}^{-1}$, $\Delta\bar{\nu} = \pm 458.7\ \text{cm}^{-1}$, $\Delta\bar{\nu} = \pm 761.7\ \text{cm}^{-1}$, and $\Delta\bar{\nu} = \pm 790.4\ \text{cm}^{-1}$. The values for these lines are from NIST; the spectrum itself is simulated.



$$\Delta\bar{\nu} = \pm 217.0\ \text{cm}^{-1},\ \Delta\bar{\nu} = \pm 313.5\ \text{cm}^{-1},$$
$$\Delta\bar{\nu} = \pm 458.7\ \text{cm}^{-1},\ \Delta\bar{\nu} = \pm 761.7\ \text{cm}^{-1},\ \text{and}\ \Delta\bar{\nu} = \pm 790.4\ \text{cm}^{-1}$$

Third, each of the Stokes lines is more intense than the corresponding anti-Stokes line.

Fourth, because we measure the shift in a peak's wavenumber relative to the source radiation, the spectrum is independent of the source radiation.

Raman spectra of Carbon Tetrachloride (CCl_4)

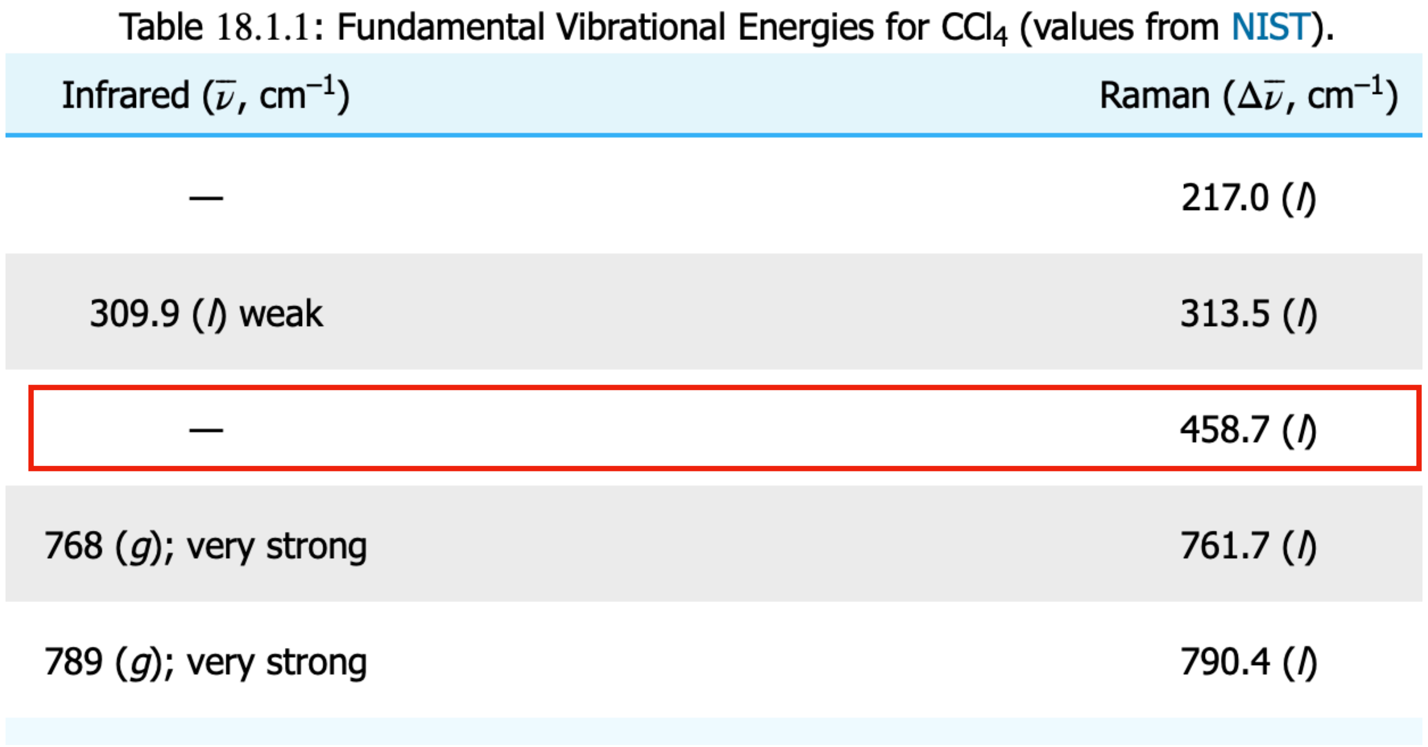
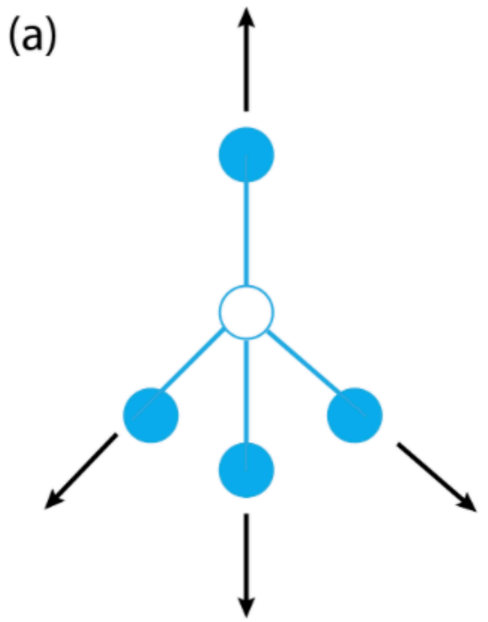


Table 18.1.1: Fundamental Vibrational Energies for CCl_4 (values from NIST).

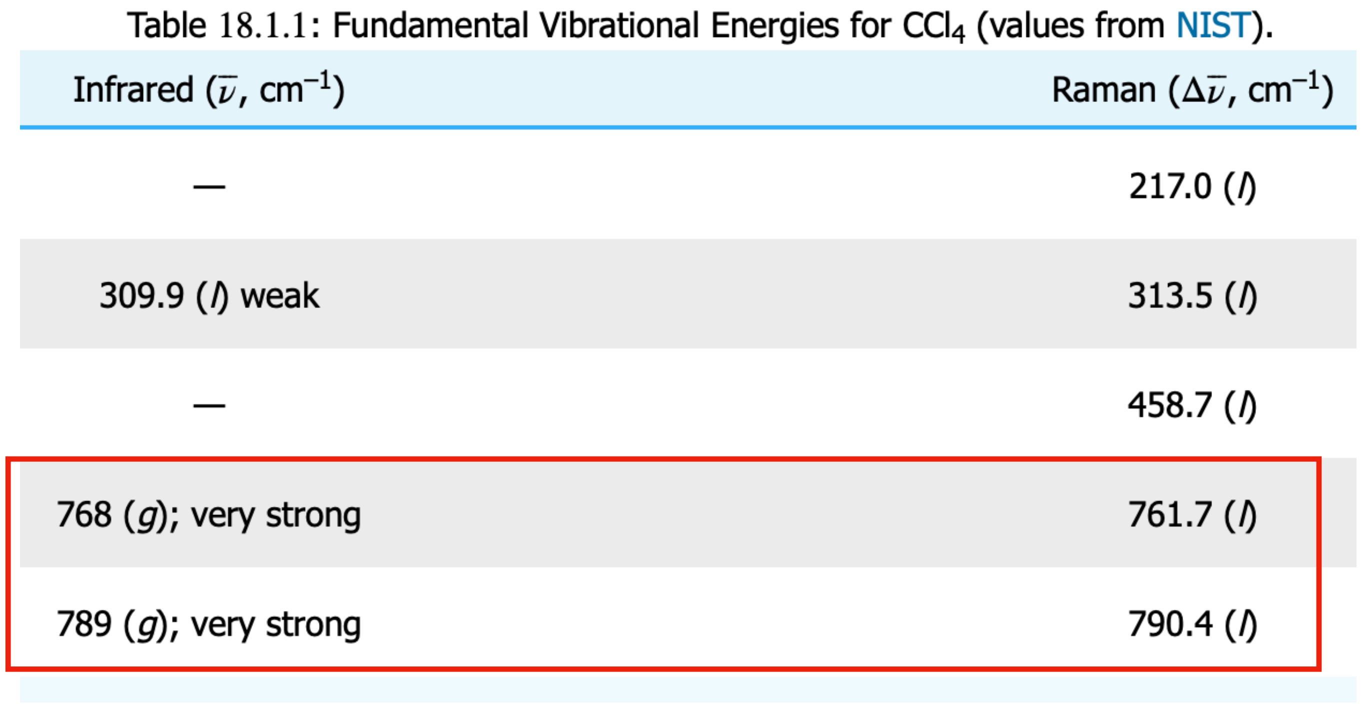
Infrared ($\bar{\nu}$, cm^{-1})	Raman ($\Delta\bar{\nu}$, cm^{-1})
—	217.0 (*l*)
309.9 (*l*) weak	313.5 (*l*)
—	458.7 (*l*)
768 (*g*); very strong	761.7 (*l*)
789 (*g*); very strong	790.4 (*l*)



symmetric stretching
IR inactive
Raman active (458.7 cm^{-1})

(a) In which all four C–Cl bond lengths increase and decrease together, means the molecule's volume increases and decreases; thus, this vibrational mode is Raman active. The symmetry of the stretching motion, however, means there is no change in the molecule's dipole moment and the vibrational mode is IR inactive.

Raman spectra of Carbon Tetrachloride (CCl_4)



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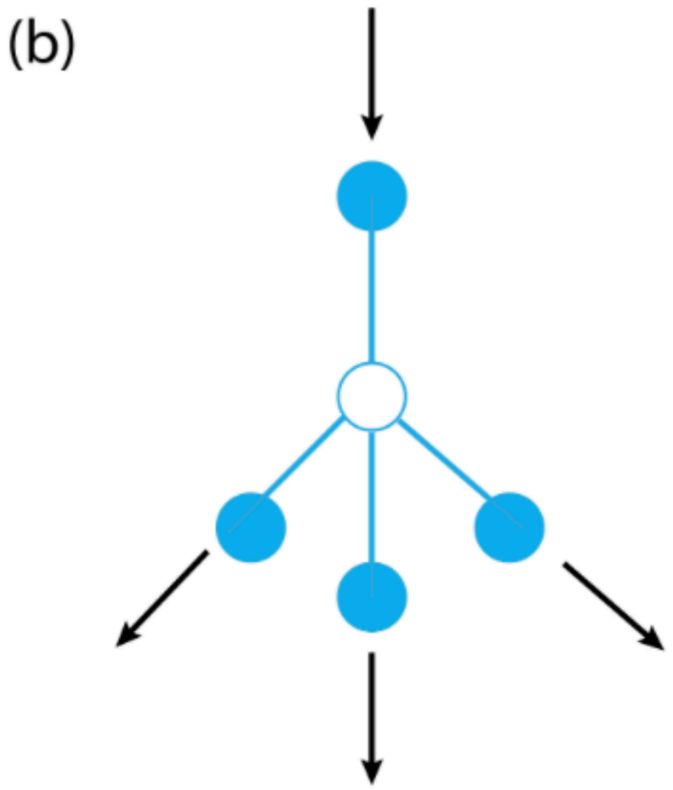
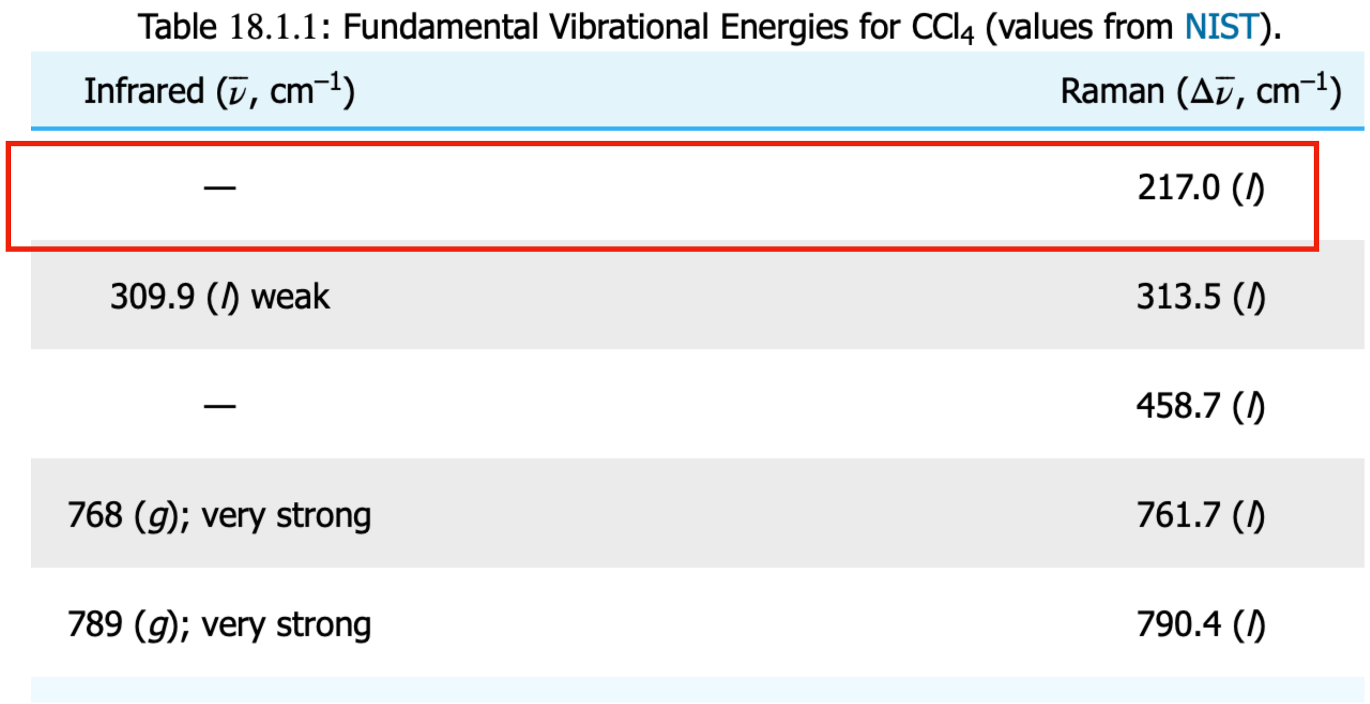


assymmetric stretching
IR active (768 cm^{-1}, 789 cm^{-1})
Raman active (761.7 cm^{-1}, 790.4 cm^{-1})

The asymmetric stretch in (b), on the other hand, is both IR and Raman active.

Raman spectra of Carbon Tetrachloride (CCl_4)



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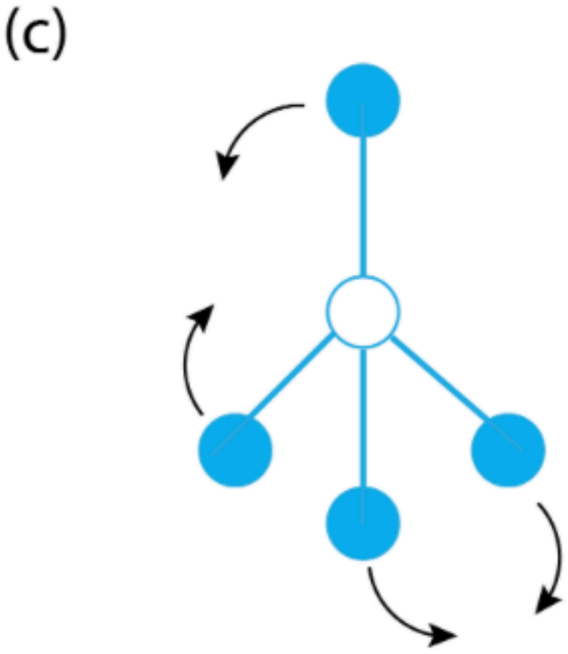

scissoring
IR inactive
Raman active (217.0 cm^{-1})

The bending motion in (c) results in the molecule becoming more or less compact in size, and is Raman active; the symmetry of the **scissoring motions**, however, means that the vibrational mode is IR inactive.

Raman spectra of Carbon Tetrachloride (CCl_4)

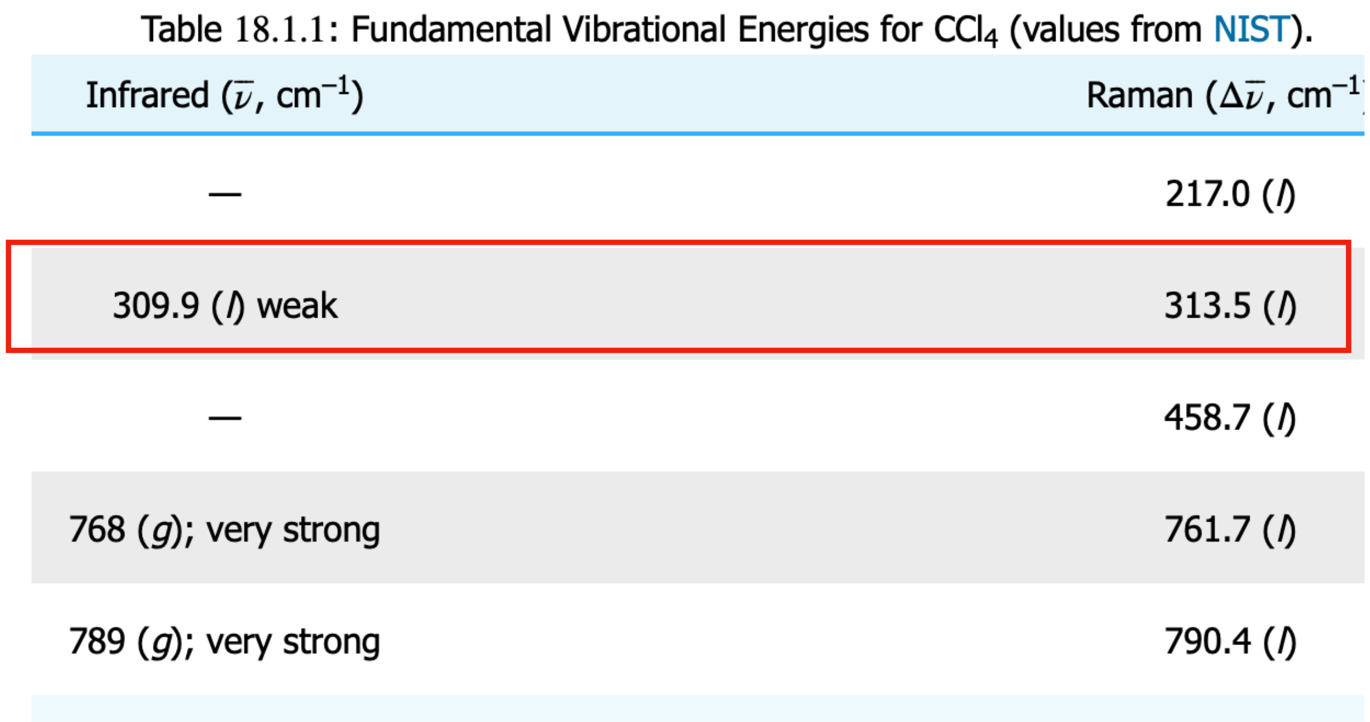

Table 18.1.1: Fundamental Vibrational Energies for CCl_4 (values from NIST).

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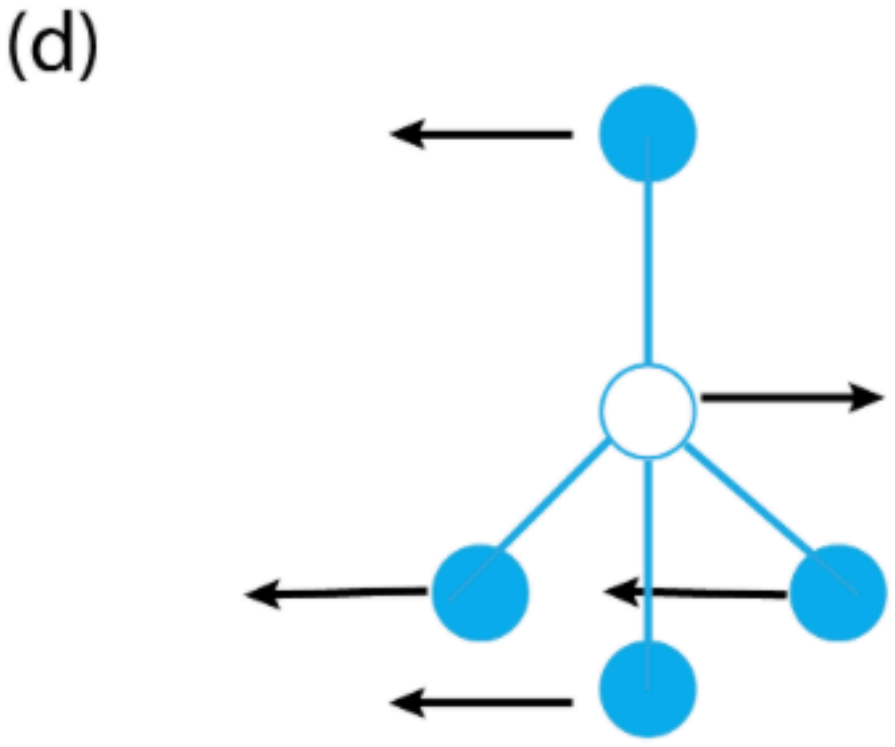
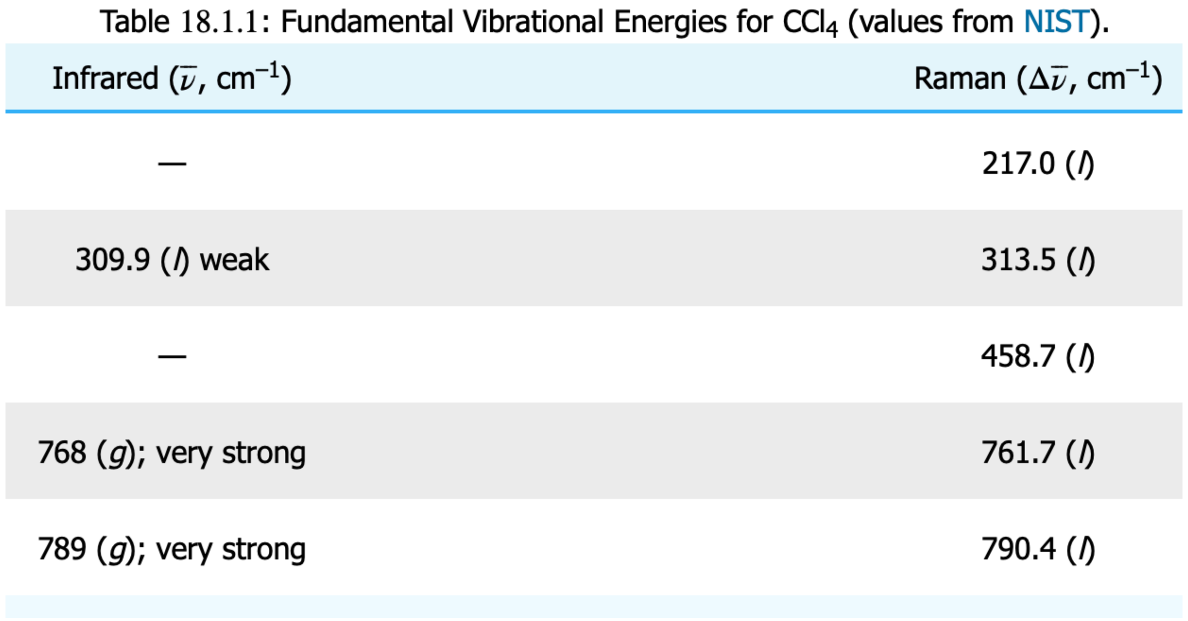
789 (*g*); very strong	790.4 (*l*)



wagging
IR active (309.9 cm^{-1})
Raman active (313.5 cm^{-1})

The bending motions in (d) are both IR and Raman active.

Raman spectra of Carbon Tetrachloride (CCl_4)



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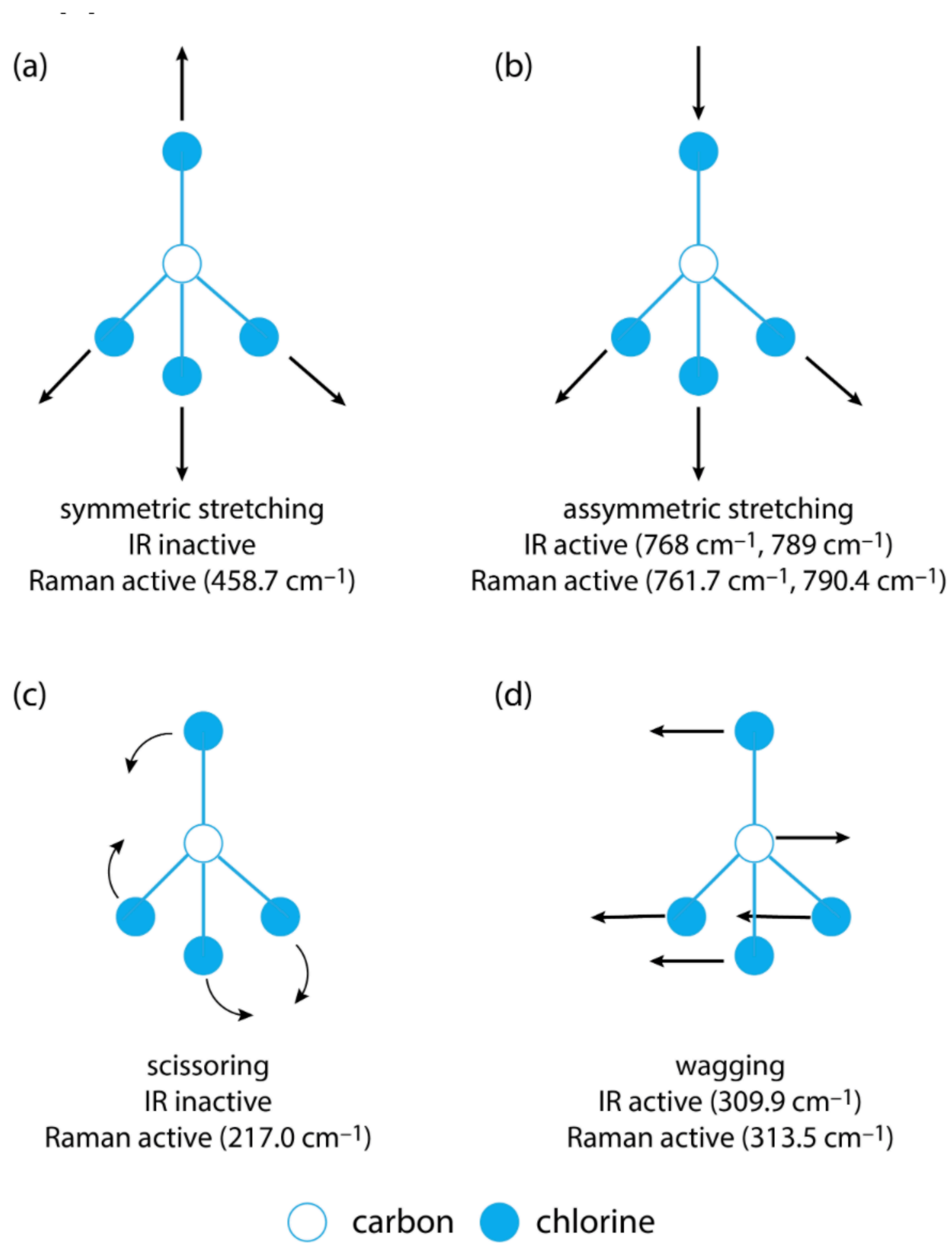


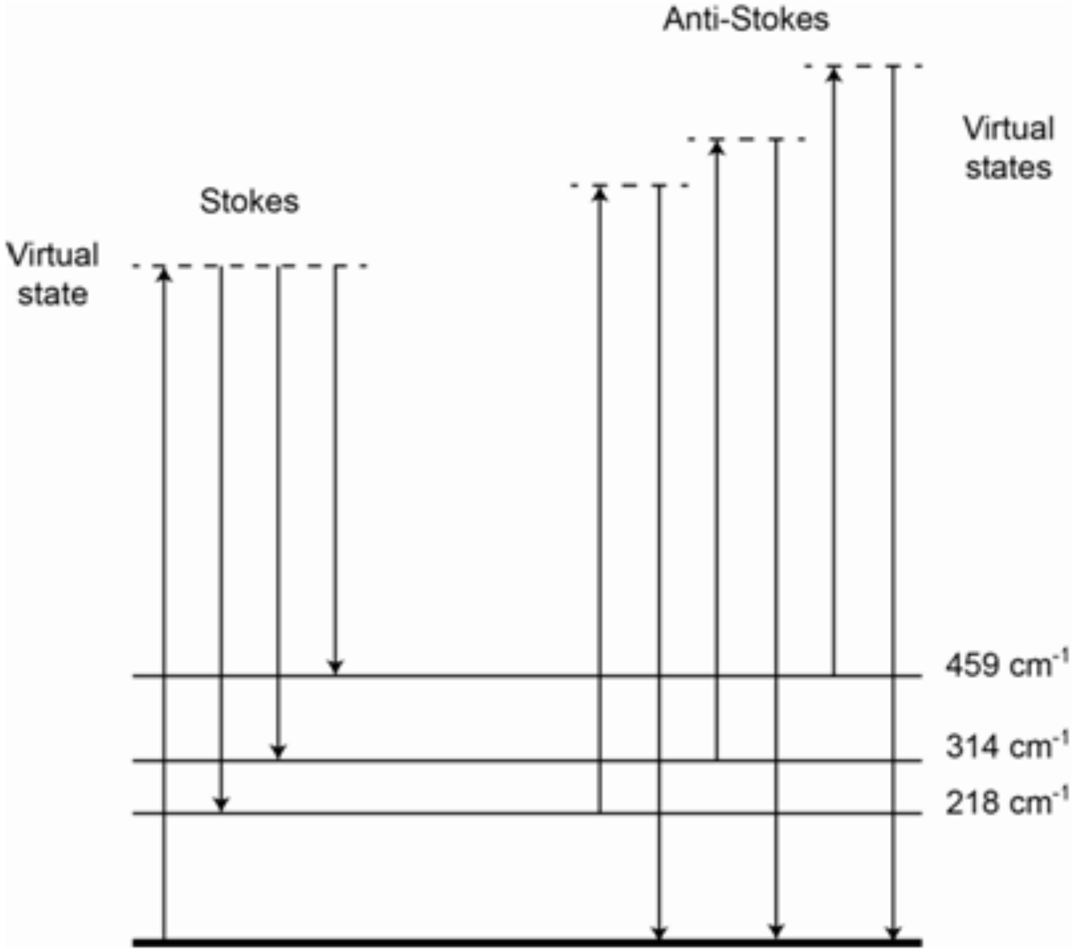
(a) symmetric stretching
IR inactive
Raman active (458.7 cm^{-1})

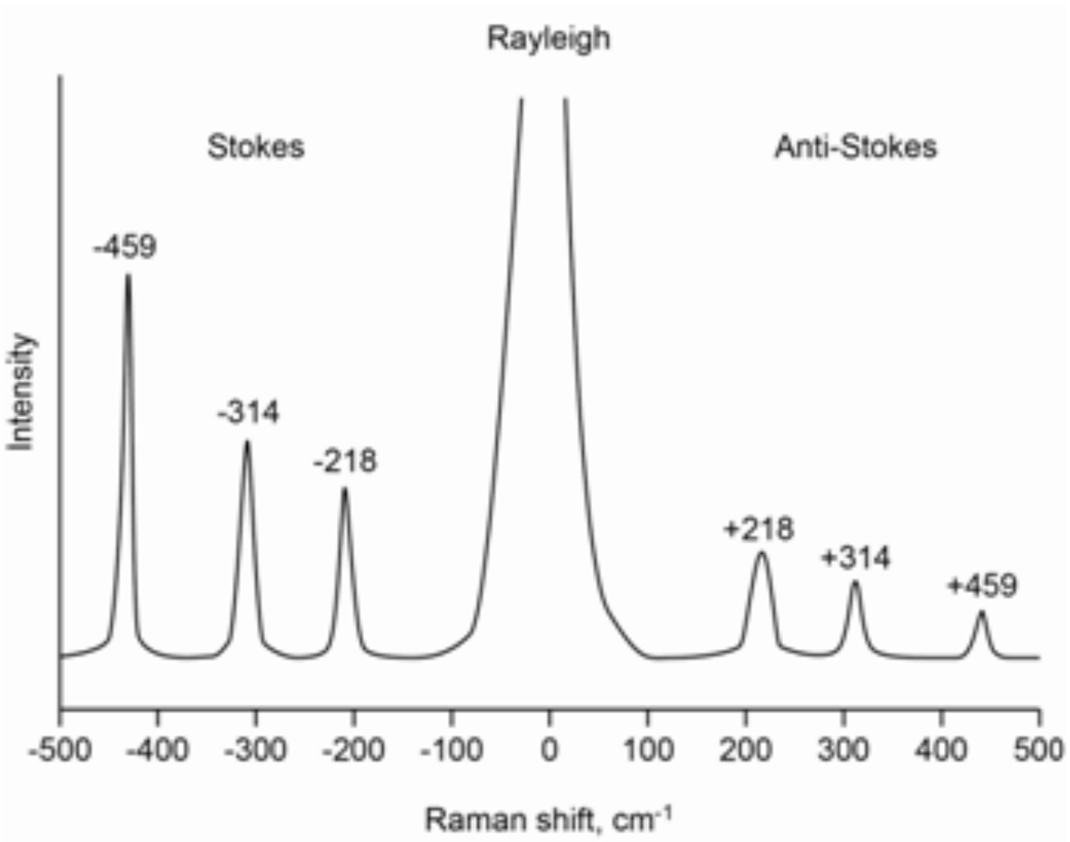
(b) assymmetric stretching
IR active (768 cm^{-1}, 789 cm^{-1})
Raman active (761.7 cm^{-1}, 790.4 cm^{-1})

(c) scissoring
IR inactive
Raman active (217.0 cm^{-1})

(d) wagging
IR active (309.9 cm^{-1})
Raman active (313.5 cm^{-1})

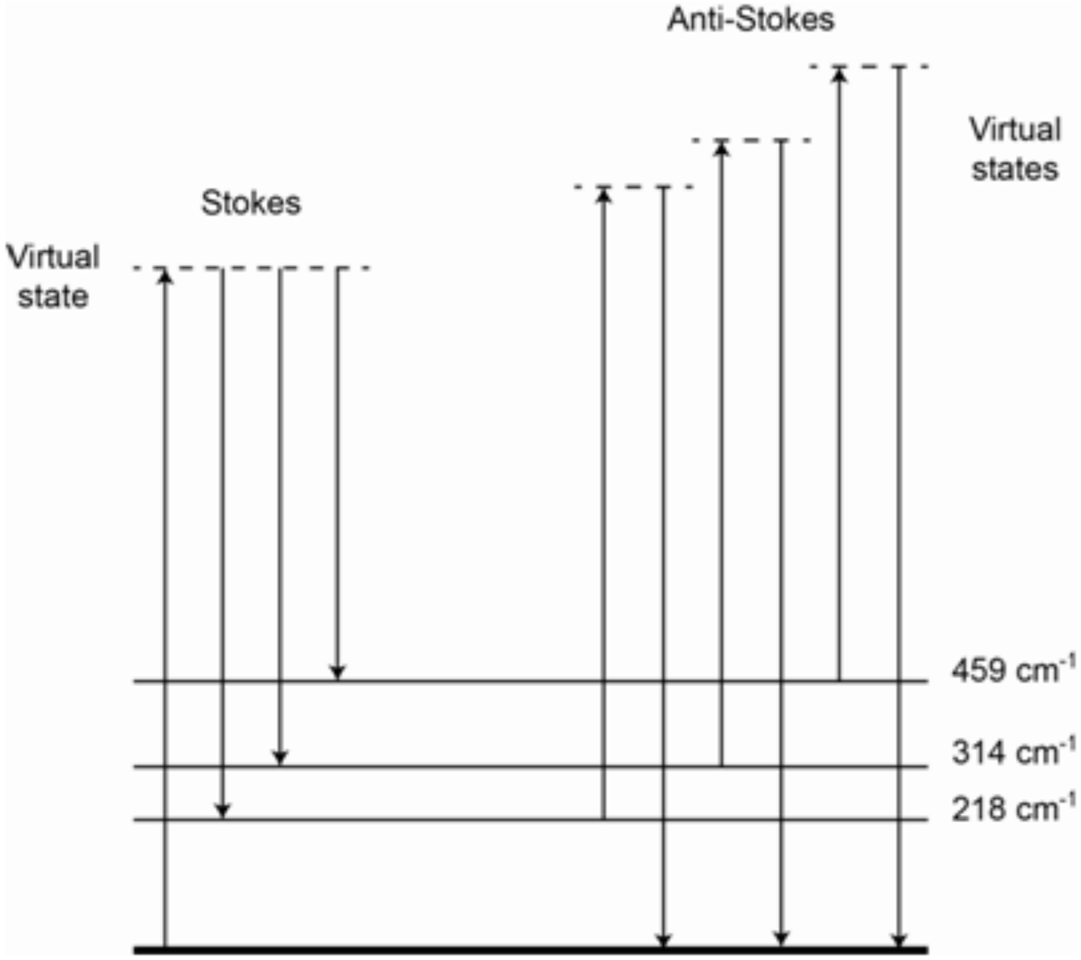
Why do the anti-Stokes lines of carbon tetrachloride have the following order of intensity: 219 > 314 > 459 cm-1?

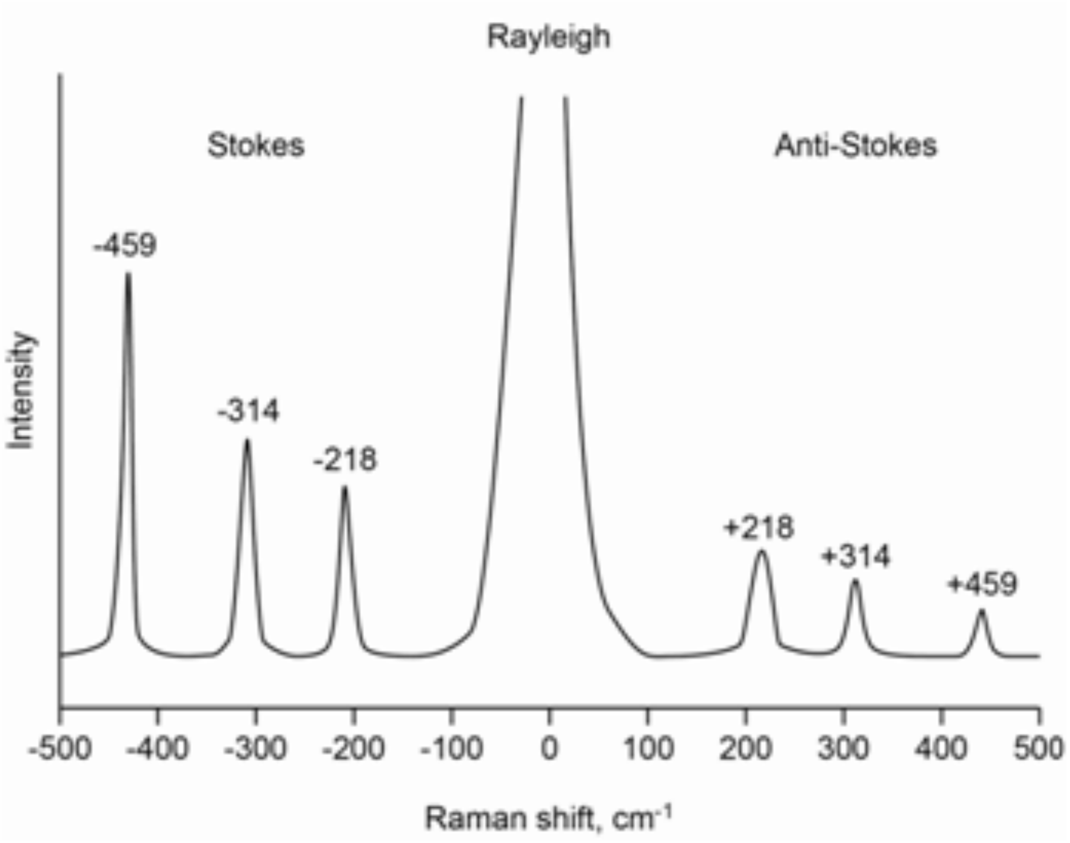




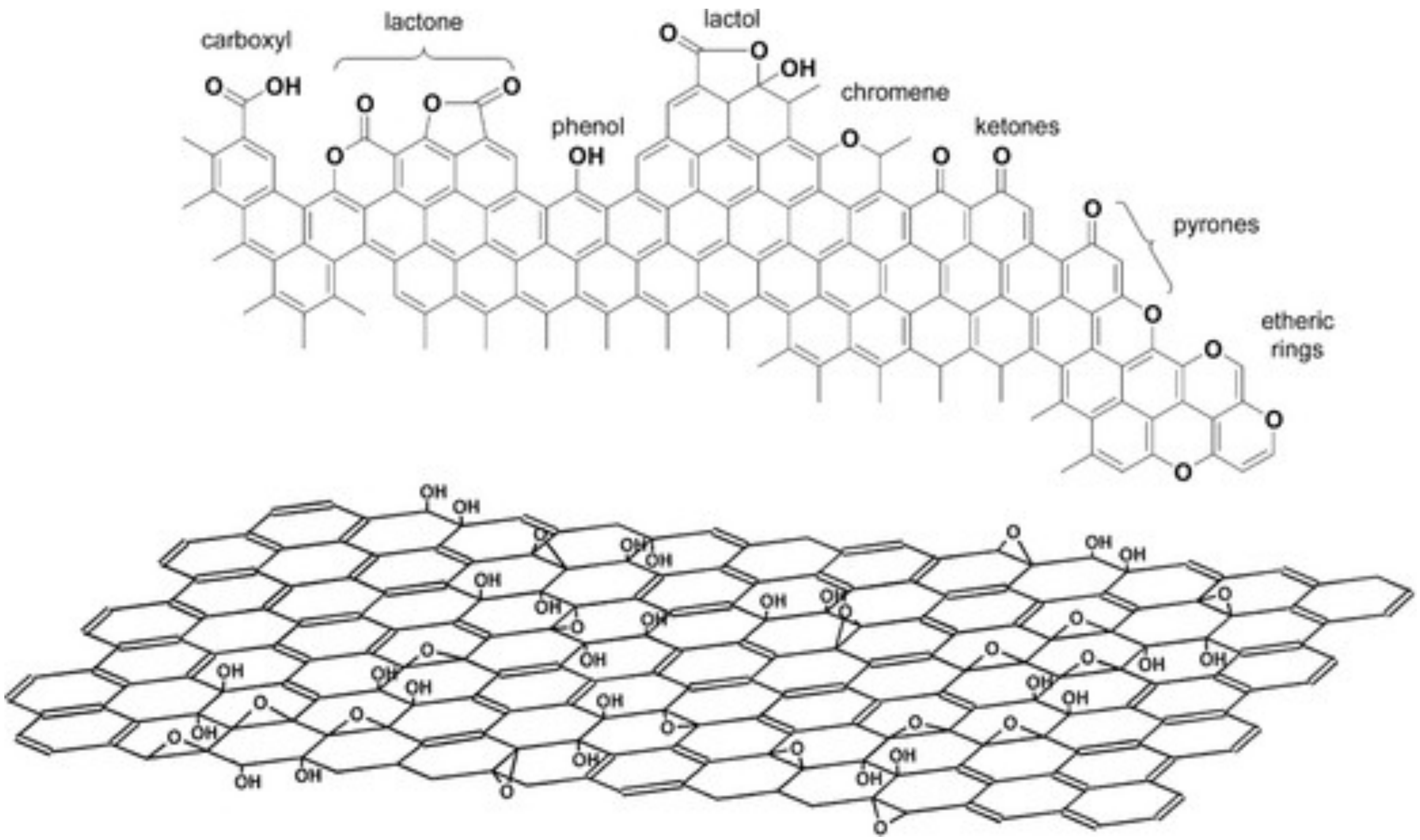
The intensity of the three anti-Stokes lines drops going from the 218 to 314 to 459 cm-1 band. **Anti-Stokes scatter requires an interaction of the incident photon with vibrationally excited molecules. Heat in the system causes some molecules to be vibrationally excited. The drop in intensity is predictable because, as the vibrational levels increase in energy, they would have lower populations** and therefore fewer molecules to produce Raman scatter at that transition.

The molecule carbon tetrachloride (CCl_4) has three Raman-active absorptions that occur at 218, 314 and 459 cm-1 away from the laser line. Draw a representation of the Raman spectrum of CCl_4 that includes both the Stokes and anti-Stokes lines.





Characterising graphene



(a) Structure of functional groups at the edges of graphene oxide.
(b) Structure of functional groups at basal graphene plane epoxide (C–O–C) and hydroxyl (C–OH) functional groups

Characterising graphene

The G-band:

It represents the planar configuration sp2 bonded carbon that constitutes graphene.

- G-band is to aid in determination of graphene layer thickness

The *G* peak is due to the bond stretching of all pairs of sp^2 atoms in both rings and chains.

- Independent of excitation laser frequency

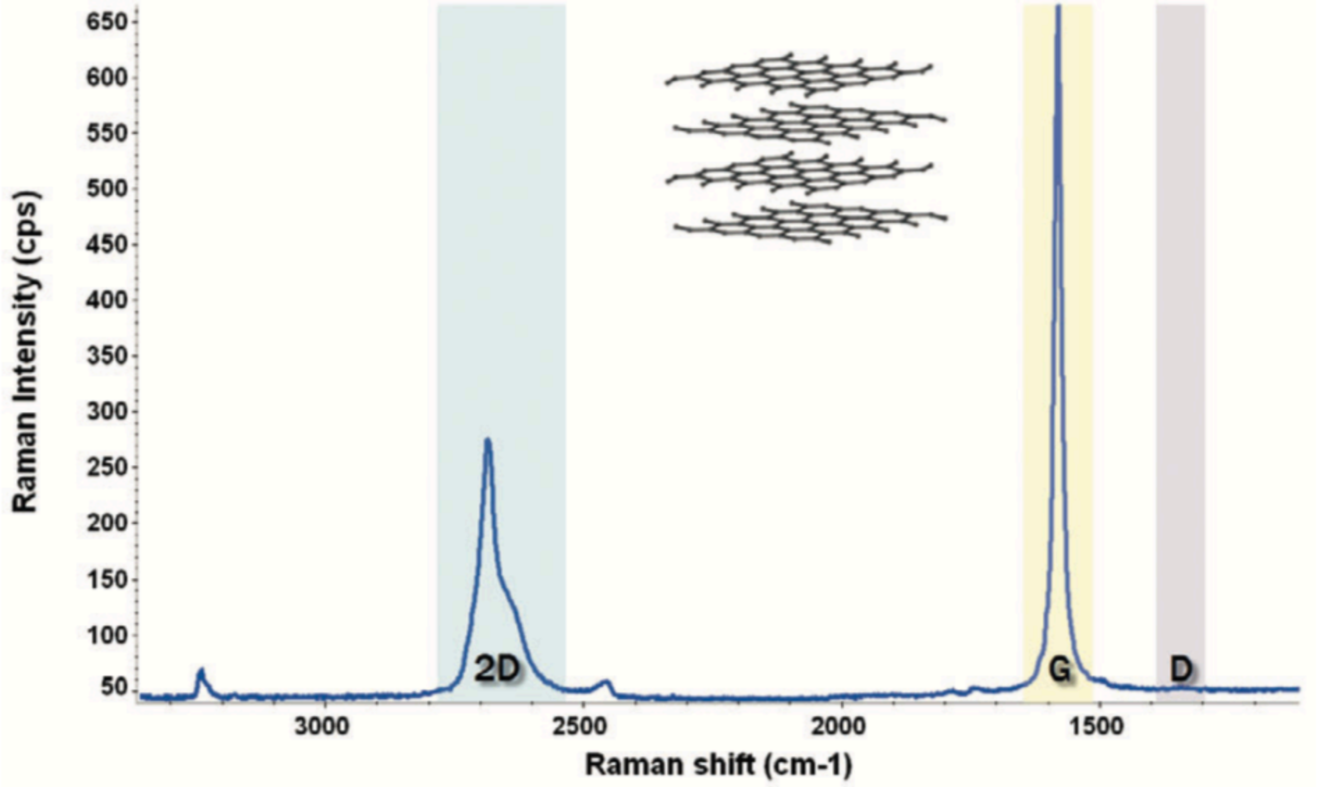
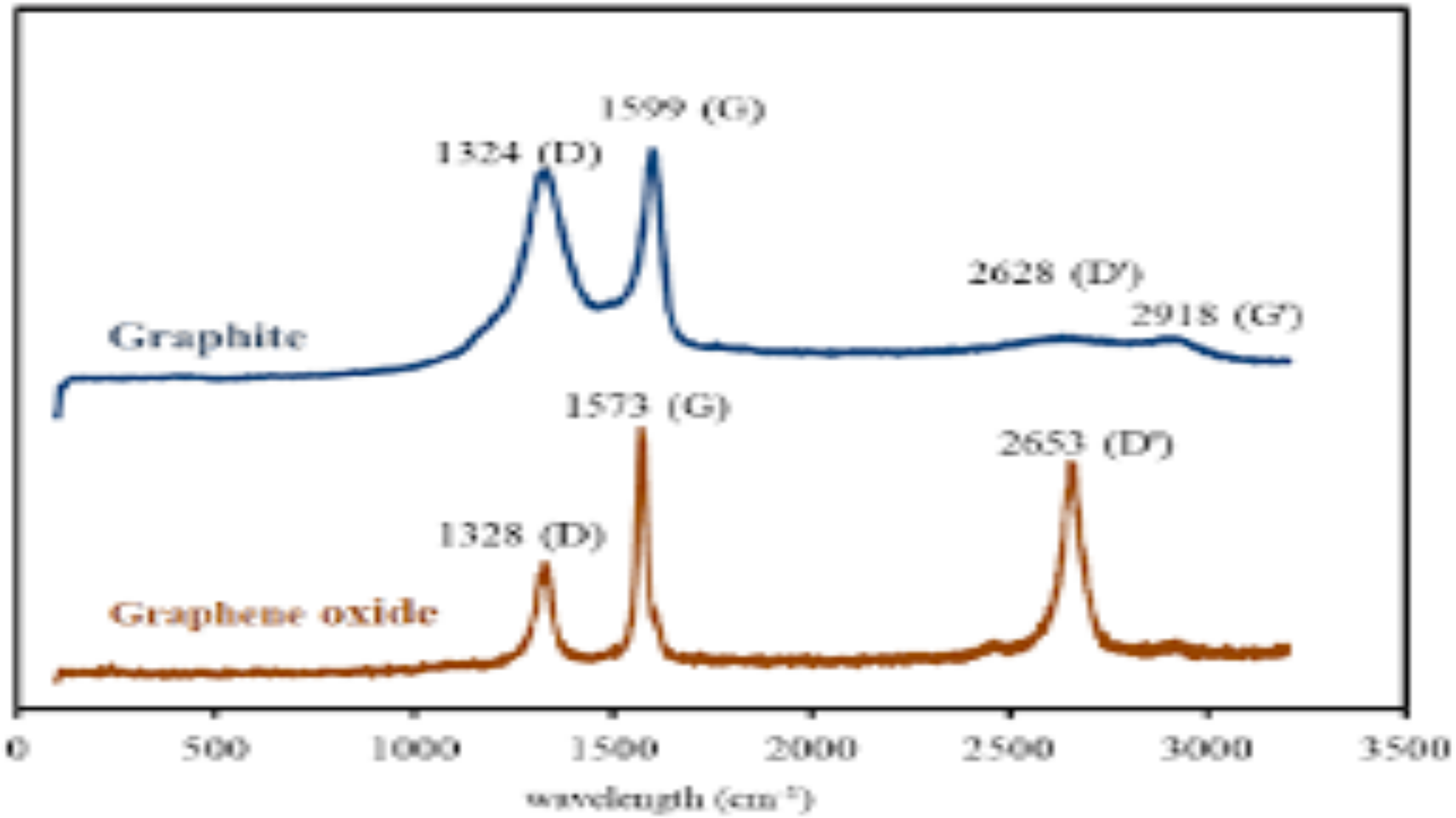


Figure 1. Raman spectrum of highly ordered pyrolytic graphite (HOPG). 633 nm excitation laser.

G band - in-plane vibrations of SP2 bonded carbon atoms
D band is due to out of plane vibrations attributed to the presence of structural defects.

Now, when you compare the spectra of graphene and graphene oxide, GO will have a higher D band. This is due to the disruption of SP2 bonds of the carbon as GO has oxidative functional groups.

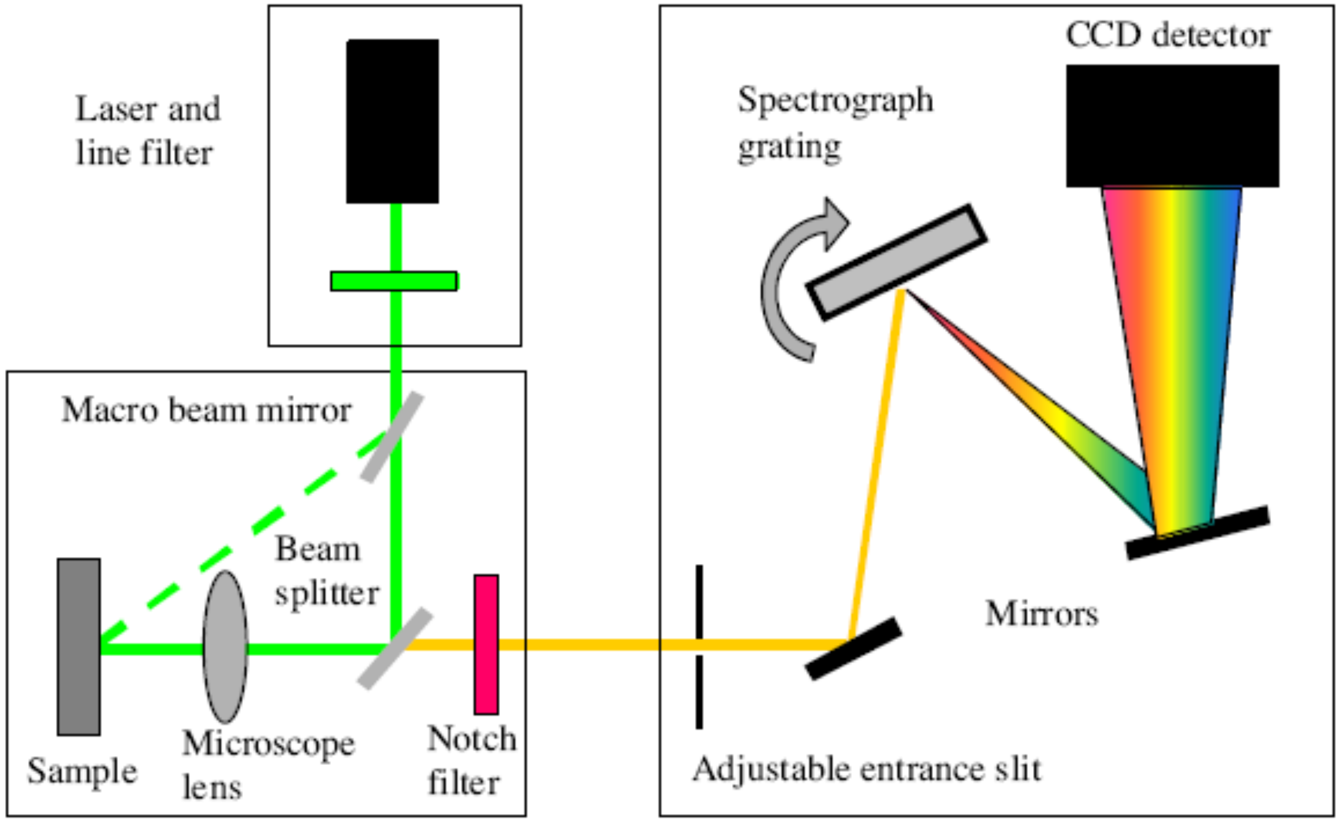


So, if the D band is higher, it means that the SP2 bonds are broken which in turn means that there are more SP3 bonds. However, D band can be present due to various other reasons. So if your D/G ratio is higher than pristine graphene, it means that there are defects. It does not mean that you have more SP3 than SP2 in the same sample. It shows that you have more SP3 in GO compared to pristine graphene.

Raman Spectrometer

Components

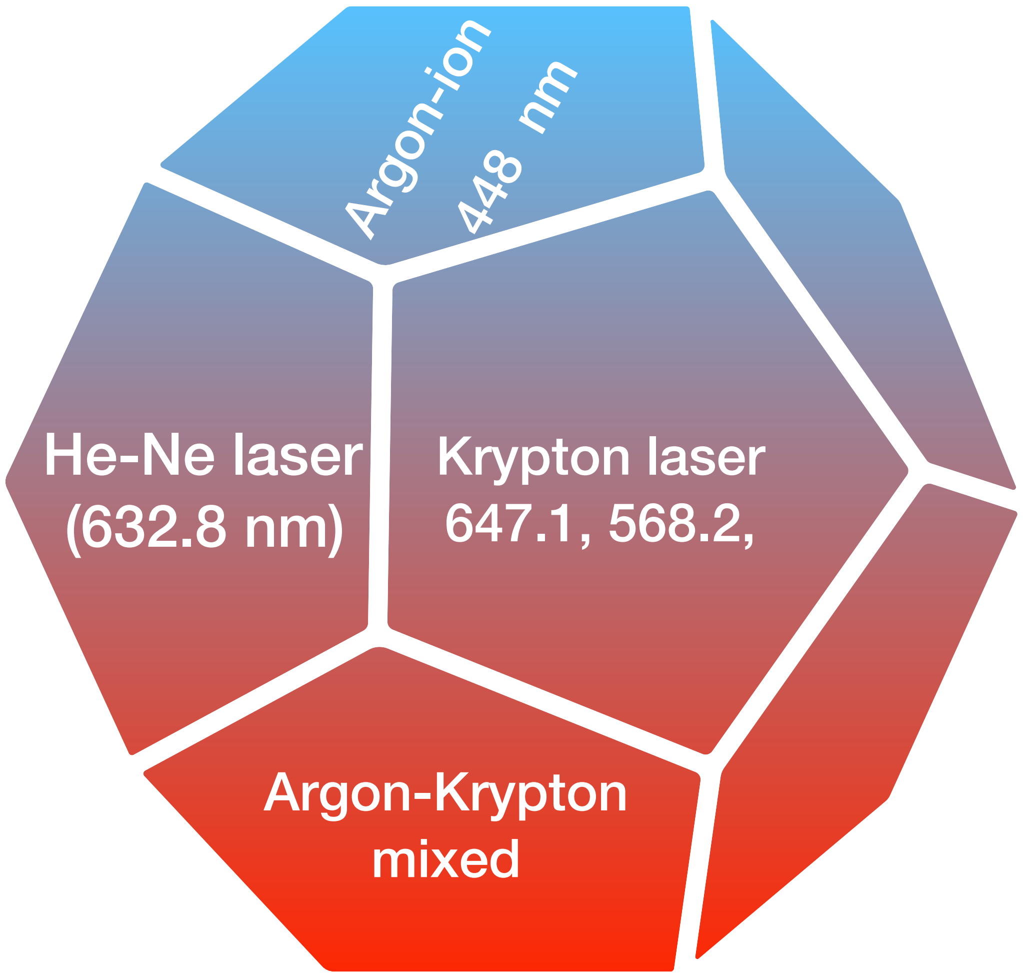
- Source
- Sample cell
- Collecting lance
- Monochromator
- CCD
- Amplifier
- Recorder



Raman spectroscopy uses intense light from a laser to probe the chemical bonds in a substance, generating a spectrum that acts as a fingerprint which can be used to characterise or identify the substance. This can be used to authenticate materials or assess their quality, and even for medical diagnostics.

Raman Spectrometer

Raman spectroscopy uses visible or near-infrared light to measure a spectrum of vibrational bonds in seconds.



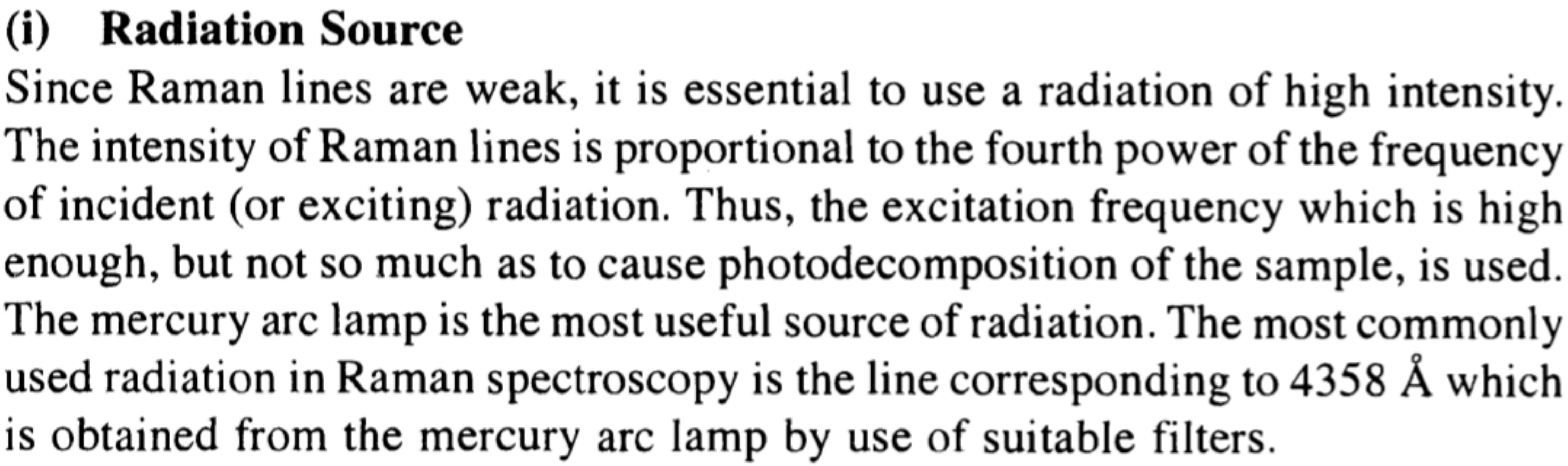
Argon-ion 448 nm

He-Ne laser (632.8 nm)

Krypton laser 647.1, 568.2,

Argon-Krypton mixed

What would be the ideal source to use for measuring Raman spectra?



(i) Radiation Source

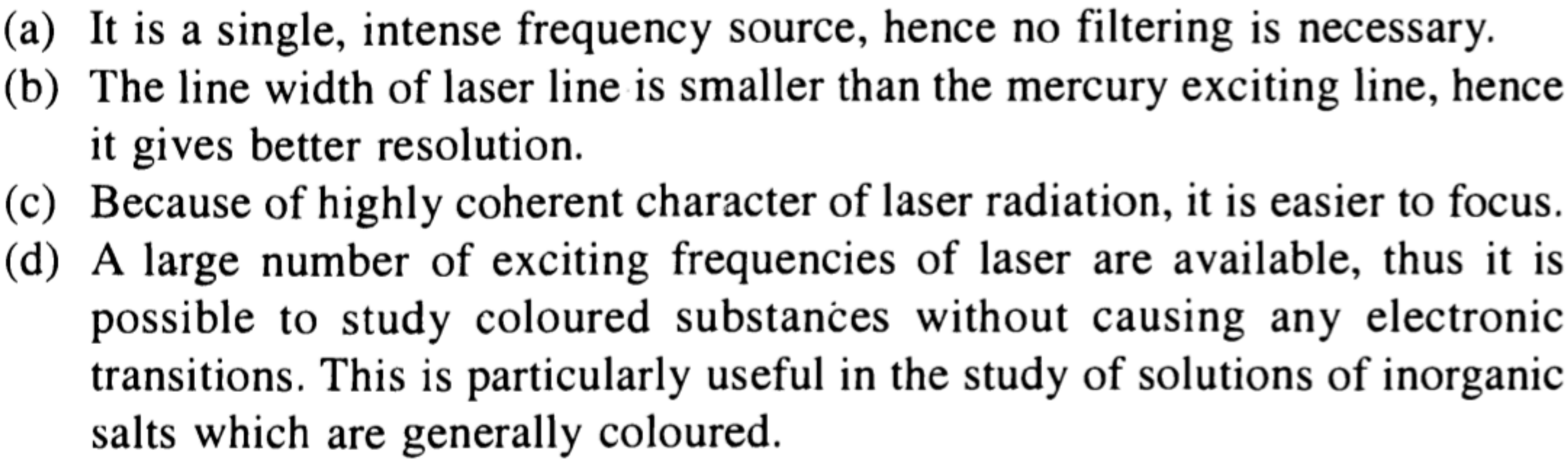
Since Raman lines are weak, it is essential to use a radiation of high intensity. The intensity of Raman lines is proportional to the fourth power of the frequency of incident (or exciting) radiation. Thus, the excitation frequency which is high enough, but not so much as to cause photodecomposition of the sample, is used. The mercury arc lamp is the most useful source of radiation. The most commonly used radiation in Raman spectroscopy is the line corresponding to 4358 Å which is obtained from the mercury arc lamp by use of suitable filters.

How the Raman technique suffer Mercury arc lamp

Before the application of Laser in Raman spectroscopy, it suffered from the following disadvantages:

- Samples had to be colourless, clear and non-fluorescent liquids.
- The low intensity of Raman lines required relatively concentrated solutions.
- Much larger volume of sample solutions were needed than that for IR spectroscopy.

Advantage of LASER

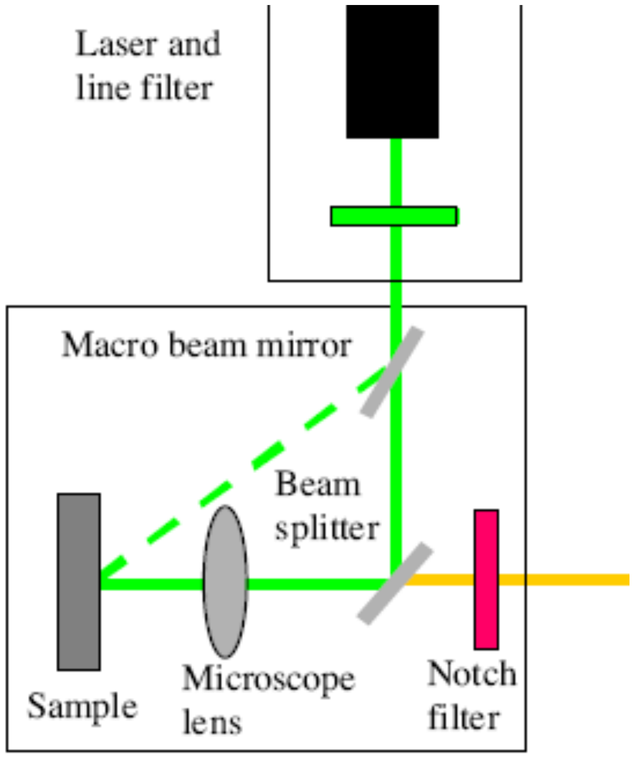


(a) It is a single, intense frequency source, hence no filtering is necessary.
(b) The line width of laser line is smaller than the mercury exciting line, hence it gives better resolution.
(c) Because of highly coherent character of laser radiation, it is easier to focus.
(d) A large number of exciting frequencies of laser are available, thus it is possible to study coloured substances without causing any electronic transitions. This is particularly useful in the study of solutions of inorganic salts which are generally coloured.

Raman Spectrometer

(ii) Filters

In case of non-monochromatic incident radiation, there will be overlapping of Raman shifts making the interpretation of the spectrum difficult. Thus, monochromatic incident radiations are necessary. Filters are used to obtain monochromatic radiation. They are generally made of nickel oxide or quartz. Sometimes, a coloured solution, e.g. aqueous solution of potassium ferricyanide or solution of iodine in carbon tetrachloride, is used as a monochromator.



A **notch-filter** is usually placed in front of the monochromator to decrease the intensity of the Rayleigh band, allowing the Raman bands to be more easily displayed. The notch filter absorbs in a narrow band of frequencies centered on the incident laser frequency, while allowing **redder** **or** **bluer** light to pass unattenuated.

(iii) Sample (Raman) Tube

Various types of sample tubes are in use for Raman spectroscopy (Fig. 4.5). The shape and size of the tube depends on the intensity of incident radiation, nature of the sample and its available amount. For gases, relatively bigger tubes are required.

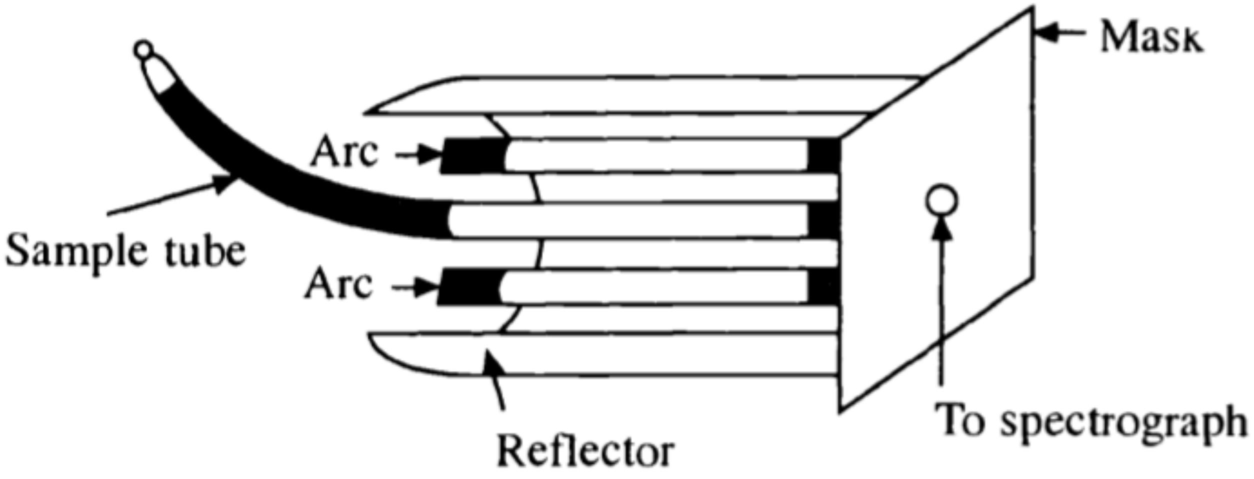


Fig. 4.5 Sample (Raman) tube

Sample preparation

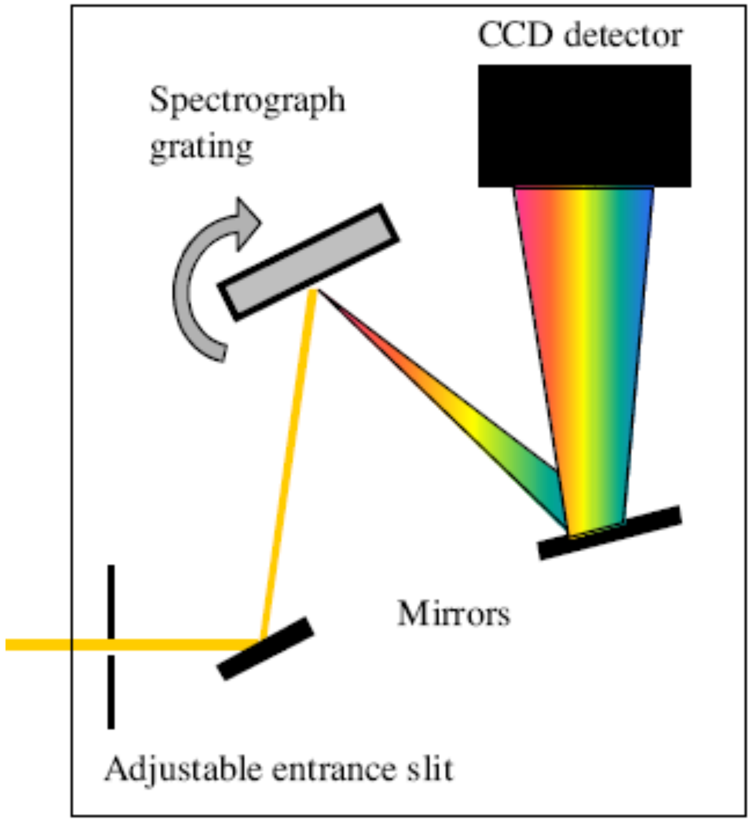
1. A narrow glass or quartz tube is filled with the sample, generally 10- 100 ml is used. Solution at least 0.1M strength is used.
2. Drop the solution onto surface of glass slide, and wait few days for the solvent evaporate. ...
3. Put the solid sample onto surface and strongly press it.
4. Squeeze the solid sample to convert into tiny solid species (maybe not powder).

Raman Spectrometer

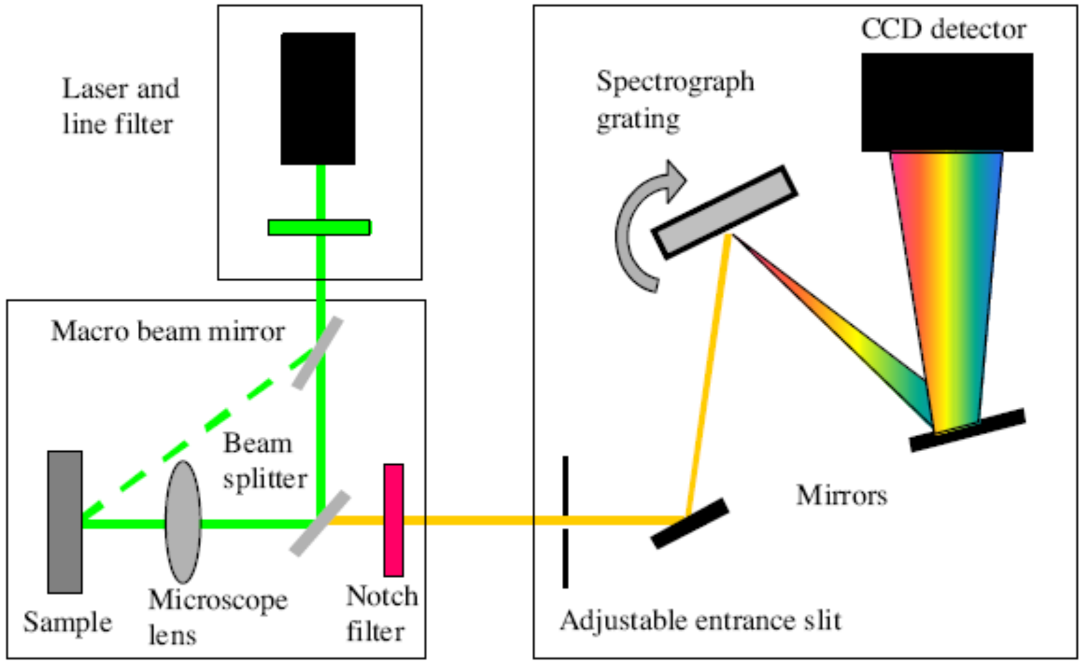
CCD detector

A charge coupled device (CCD) is the most commonly used detector in Raman microscopy. It is a **highly sensitive photon detector**, and an image is constructed from the signals collected from the pixels, which are discrete small sensitive regions on the detector surface.

Electron multiplied detectors (EMCCD) are also used and offer sensitivity at up to 50 times that of conventional silicon CCD detectors. For measurements in the near IR region, CCD detectors are not sufficiently sensitive, so that InGaAs array detectors are used instead.



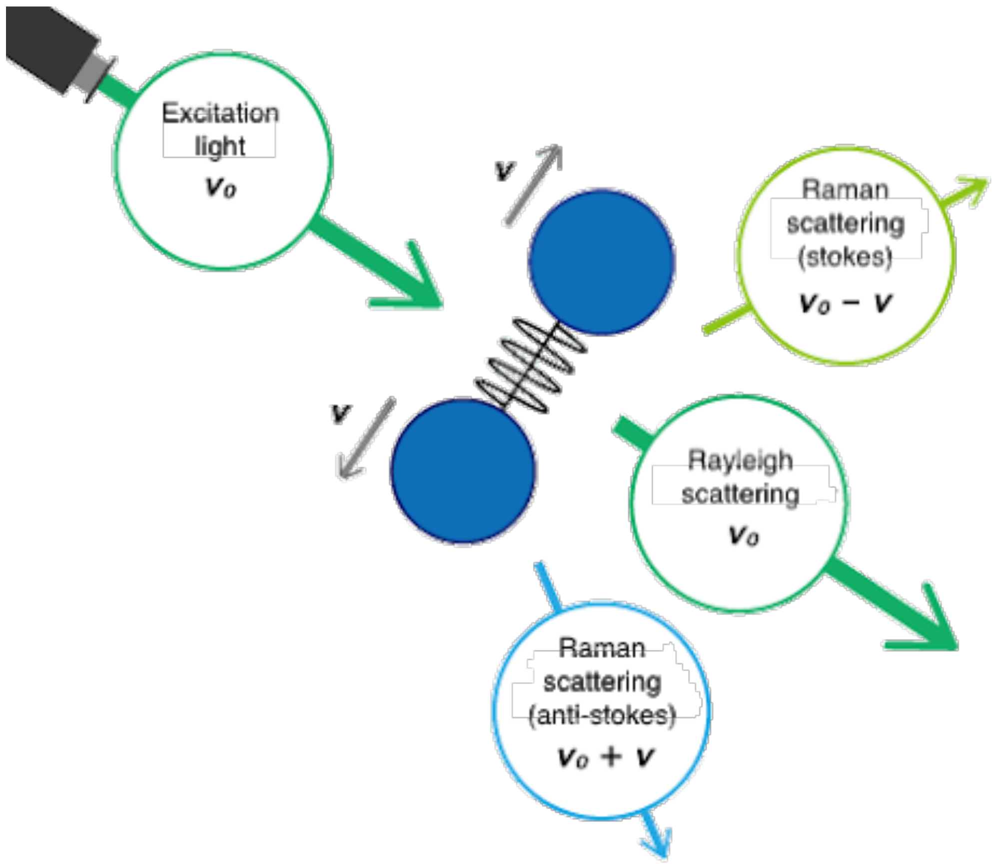
What effect would raising the temperature have on the intensity of Stokes and anti-Stokes lines?



Raising the temperature would decrease the population of the ground state and increase the population of higher energy vibrational states. **Therefore, with increased temperature, the intensity of the Stokes lines would decrease and the intensity of the anti-Stokes lines would increase.** However, the Stokes lines would still have higher intensity than the anti-Stokes lines.

Because scatter occurs in all directions, the scattered photons are measured at 90 degree to the incident radiation. Also, Raman scatter is generally a rather unfavourable process resulting in a weak signal.

Application of Raman Spectra



Carbon materials

Art Conservation and Cultural

Materials science and researching new materials

Forensics

Pharmaceuticals

Energy Technology

Life Sciences

Application of Raman Spectra

Nature of Chemical Bond

$$\bar{\nu} = \frac{1}{2\pi c}\sqrt{\frac{f}{\mu}}$$

The greater the bond strength, higher is its vibrational frequeney.

The vibrational frequeney of a molecule containing light atoms is higher than that containing heavier atoms.

The values of vibrational frequencies of H2, N2, 02, HCl, HBr and HI obtained from their Raman spectra are 4156, 2992, 2331, 2880, 2558 and 2233 cm-1, respeetively.

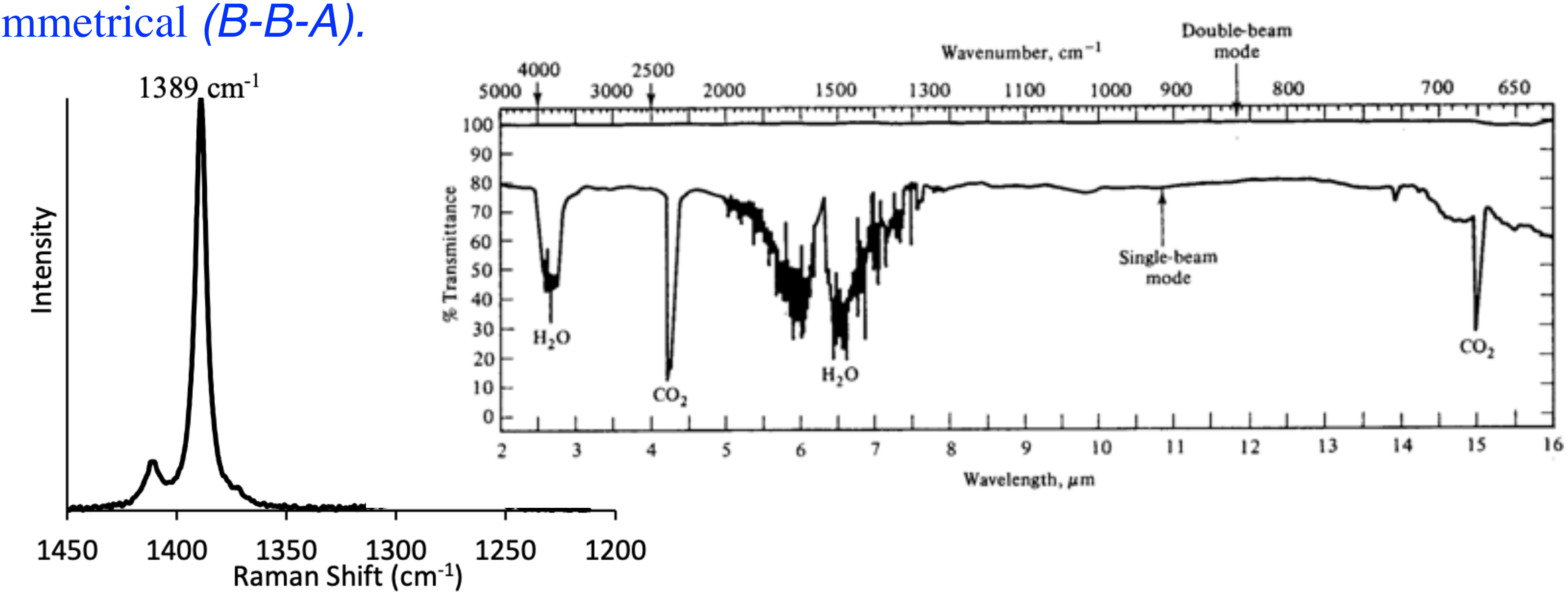
Covalent diatomic molecules show intense Raman lines, whereas no Raman lines appear in ease of electrovalent diatomic molecules.

The intensity of Raman lines essentially depends on the extent to which the polarizability is affected by the oscillations. In covalent molecules, the bonding electrons are common to the two nuclei, thus the polarizability is considerably changed by nuclear oscillations resulting in intense Raman lines. On the other hand, in electrovalent molecules, bonding electrons are transferred from one nucleus to the other during the formation of the molecules. Thus, the polarizability of the molecule is little affected by nuclear oscillations, and hence no Raman lines will appear.

Application of Raman Spectra

Structure of Triatomic molecule

Whether AB2 molecule is linear or not and, if linear, whether it is symmetrical *(B-A-B)* or asymmetrical *(B-B-A).*



It shows two very strong absorption bands at 2349 and 668 cm-1 in its IR spectrum. Since none of these bands is present in both the spectra, the molecule of CO2 must have a center of symmetry according to the rule of mutual exclusion.For triatomic molecules, this observation shows that the molecule is linear and symmetric.

Carbon disulphide (CS2) is another example of this type.

Structure of Triatomic molecule(N2O)

The three fundamental frequencies of N2O are 2224, 1285 and 589 cm-1.

Raman: 2224, 1285 cm-1

Thus, according to the rule of mutual exclusion, the molecule has no center of symmetry, i.e. it does not have the structure N - 0 - N , because two bands are common to both its IR and Raman spectra.

Hence, N2O has the unsymmetrical structure N - N - 0 . This conclusion is confirmed by the rotational Raman spectrum which consists of both (odd and even) sets of lines without any alternation in intensity. Other molecules of this type are HCN, CICN, BrCN etc.

Structure of Triatomic molecule(H2O)

The IR spectrum of water exhibits very strong bands at 3756 and 1595 cm-1. In the Raman spectrum, two bands have been recorded at 3605 and 1665 cm-1 which roughly correspond to the IR bands. This confirms that water has a symmetrical and bent structure

Application of Raman Spectra

Unlike inorganic compounds, organic compounds have less elements mainly carbons, hydrogens and oxygens. And only a certain function groups are expected in organic spectrum. Thus, Raman and IR spectroscopy are widely used in organic systems. Characteristic vibrations of many organic compounds both in Raman and IR are widely studied and summarised in many literature.

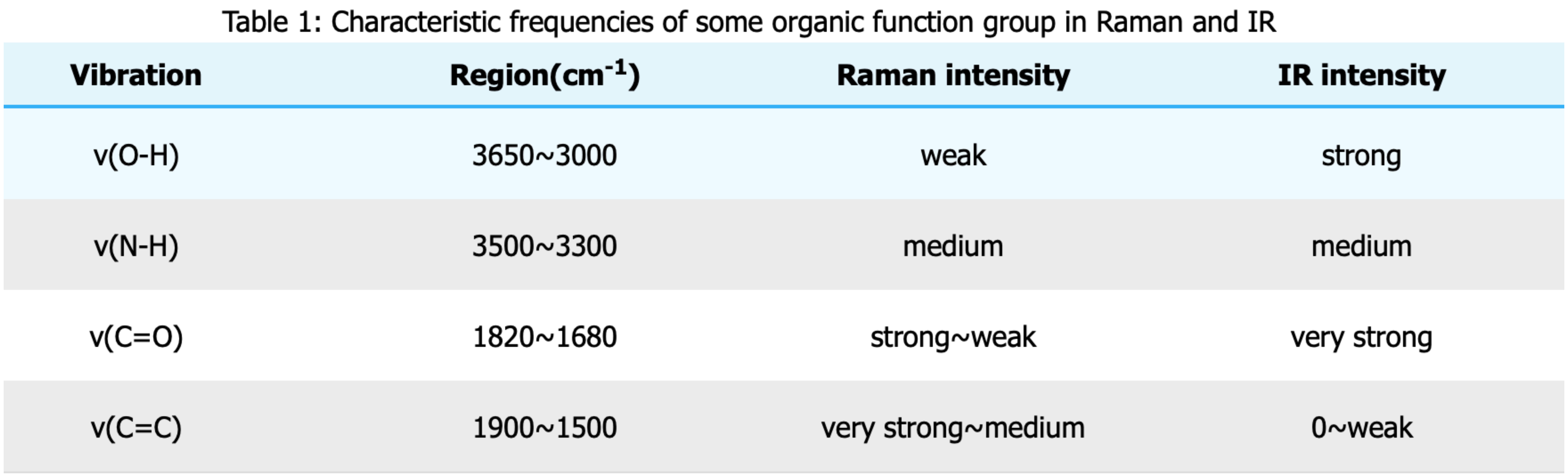


Table 1: Characteristic frequencies of some organic function group in Raman and IR

Vibration	Region(cm^{-1})	Raman intensity	IR intensity
v(O-H)	3650~3000	weak	strong
v(N-H)	3500~3300	medium	medium
v(C=O)	1820~1680	strong~weak	very strong
v(C=C)	1900~1500	very strong~medium	0~weak

Raman spectroscopy has considerable advantages over IR in inorganic systems

First, since the laser beam used in RS and the Raman-scattered light are both in the visible region, glass (Pyrex) tubes can be used in RS. On the other hand, glass absorbs infrared radiation and cannot be used in IR. However, some glass tubes, which contain rare earth salts, will gives rises to fluorescence or spikes. Thus, using of glass tubes in RS still need to be careful.

Secondly, since water is a very weak Raman scatter but has a very broad signal in IR, aqueous solution can be directly analyzed using RS.

Difficulty of Raman Spectroscopy

The main difficulty of Raman spectroscopy is to detect the Raman scattering by filtering out the strong Rayleigh scattering. In order to reduce the intensity of the Rayleigh scattering, multiple monochromator are applied to selectively transmit the needed wave range. An alternative way is to use Rayleigh filters. There are many types of Rayleigh filters. One common way to filter the Rayleigh light is by interference.

Advantage of RS over IR

Raman Spectroscopy can be used in aqueous solutions (while water can absorb the infrared light strongly and affect the IR spectrum).

Because of the different selection rules, vibrations inactive in IR spectroscopy may be seen in Raman spectroscopy. This helps to complement IR spectroscopy.

There is no destruction to the sample in Raman Spectroscopy. In IR spectroscopy, samples need to disperse in transparent matrix. For example grind the sample in solid KBr. In RS, no such destructions are needed.

Glass vials can be used in RS (this should only work in the visible region. If in UV region, glass is not applicable because it can strongly absorb light too.)

Raman Spectroscopy needs relative short time. So we can do Raman Spectroscopy detection very quickly.

Solved Problem

The carbonyl stretch for ketones is active in both IR and Raman spectroscopy. Assume a carbonyl stretch occurs at 1800. cm^{-1}. Calculate the wave lengths of the Stokes and anti-Stokes transitions in the Raman spectrum assuming laser excitation using a helium-neon laser at 632.8 nm.

Answer: The plan is to convert to wave numbers to find the transitions and then finally to convert back to wave lengths.

The laser excitation is at: $\tilde{\nu} = 1/\lambda = \dfrac{1}{632.8\ \text{nm}\ (1\text{x}10^{-9}\ \text{m}/1\text{nm})(100\ \text{cm}/1\ \text{m})} = 15803.\ \text{cm}^{-1}$

The Stokes transition is at 15803. cm^{-1} – 1800. cm^{-1} = 14003 cm^{-1}
Converting to meters and then inverting gives the wave length of the transition:

$$\lambda = 1/\tilde{\nu} = \frac{1}{14003\ \text{cm}^{-1}(100\ \text{cm}/1\ \text{m})} = 7.141\text{x}10^{-9}\ \text{m} = 714.1\ \text{nm} \qquad \text{(Stokes)}$$

The anti-Stokes transition is at 15803. cm^{-1} + 1800. cm^{-1} = 17603 cm^{-1}
Converting to meters and then inverting gives the wave length of the transition:

$$\lambda = 1/\tilde{\nu} = \frac{1}{17603\ \text{cm}^{-1}(100\ \text{cm}/1\ \text{m})} = 5.6808\text{x}10^{-9}\ \text{m} = 568.1\ \text{nm} \qquad \text{(anti-Stokes)}$$

Which of the following molecules give vibrational Raman spectra? N2, O2, NO, CH, CO, CO2, N2O, and SO2.

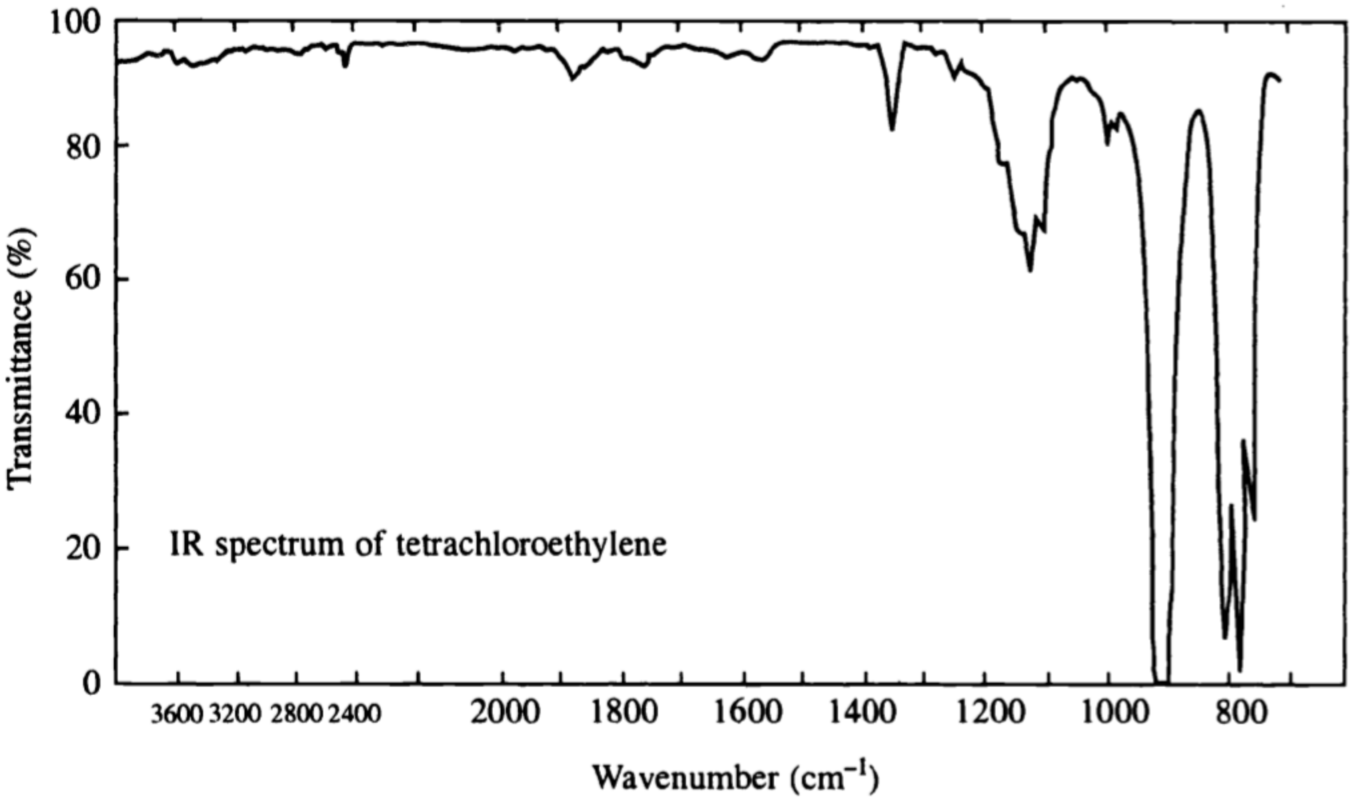
The plan is to note the molecules that have a center of symmetry, that is have an inversion center. Molecules with a center of symmetry are centrosymmetric. The exclusion rule is then applied.

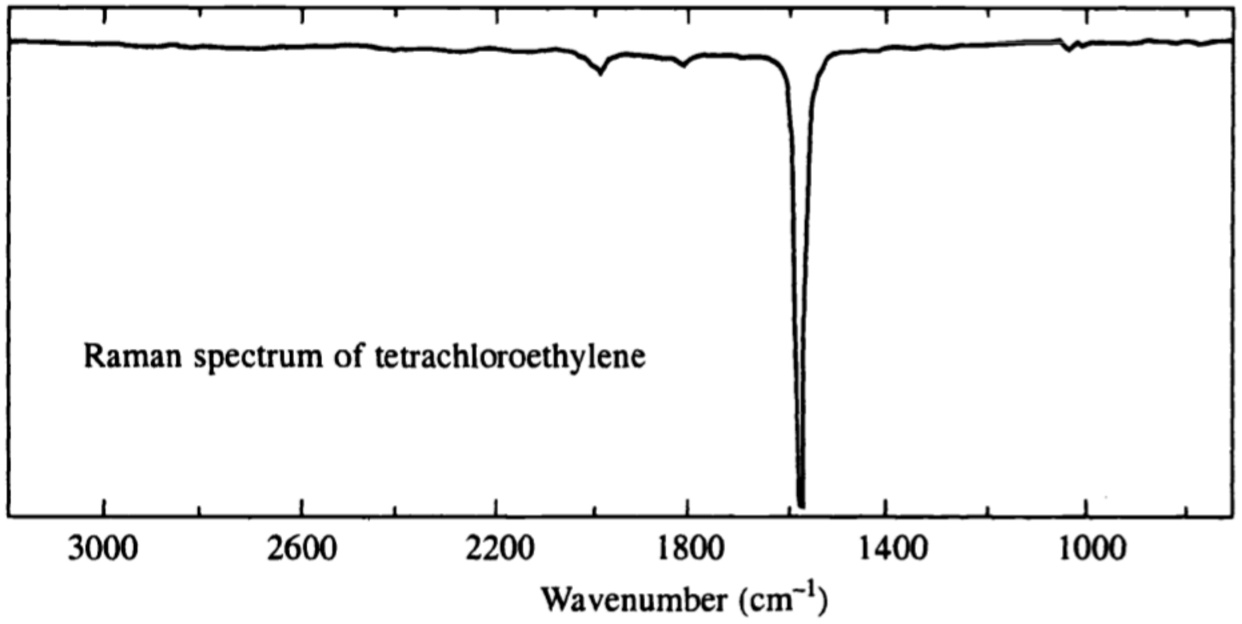
The molecules with a centre of symmetry are N2, O2, and CO2. No normal mode of a centrosymmetric molecule is both Raman and IR active. Since the homonuclear diatomics and the symmetric stretch of CO2 are IR forbidden, the stretches must be Raman active.

For the heteronuclear diatomic, the stretch is both Raman and IR active. Remember that the polarizability is a function of the volume of the molecule. As a result for the heteronuclear diatomics, the polarizability and dipole moment both change during the vibration. Therefore, NO, CH, and CO are Raman active.

All normal modes for asymmetric linear triatomics and bent triatomics are Raman active, so N2O and SO2 are Raman active.

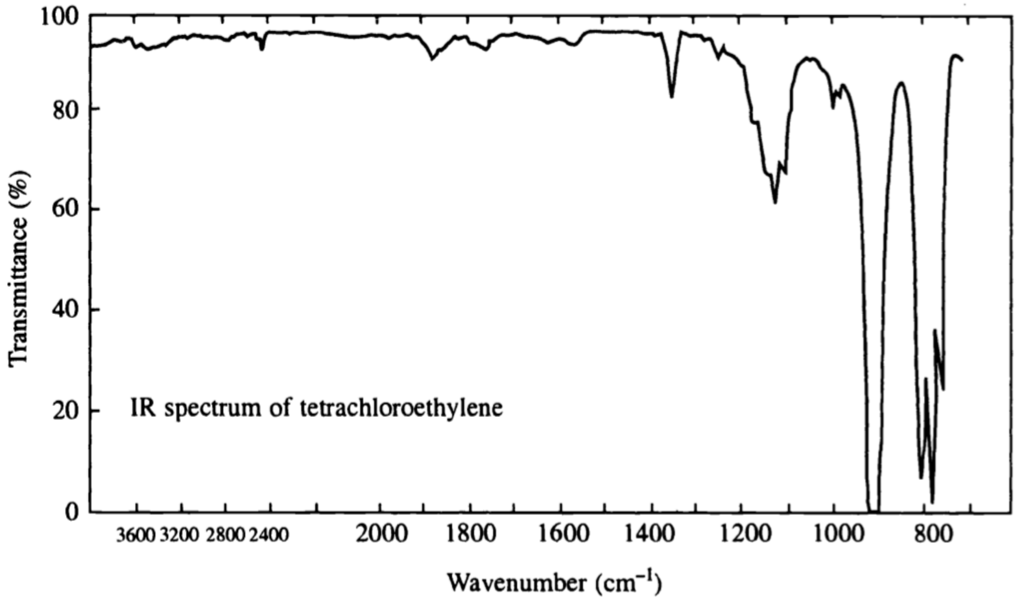
The following figure illustrate IR and Raman spectra of tetrachloroethylene. What conclusion can be drawn about the structure of the molecule?

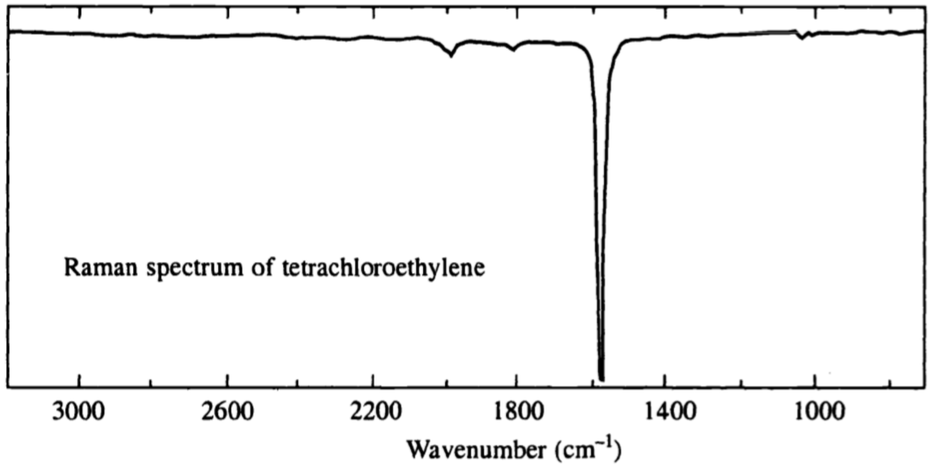




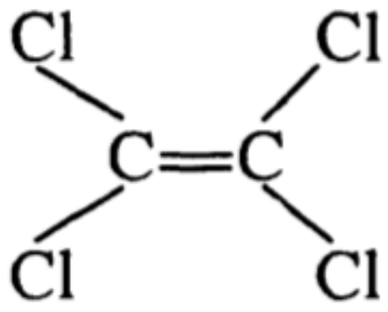
A compound having molecular formula shows IR and Raman bands but none of these bands is common to both the spectra. Assign the structure to the compound.

A compound having molecular formula shows IR and Raman bands but none of these bands is common to both the spectra. Assign the structure to the compound.





Solution. It is clear from the IR and Raman spectra of tetrachloroethylene that there is no band common to both of these spectra. Thus, according to rule of mutual exclusion, it can be concluded that tetrachloroethylene has a center of symmetry and planar structure:



Atmospheric Sample