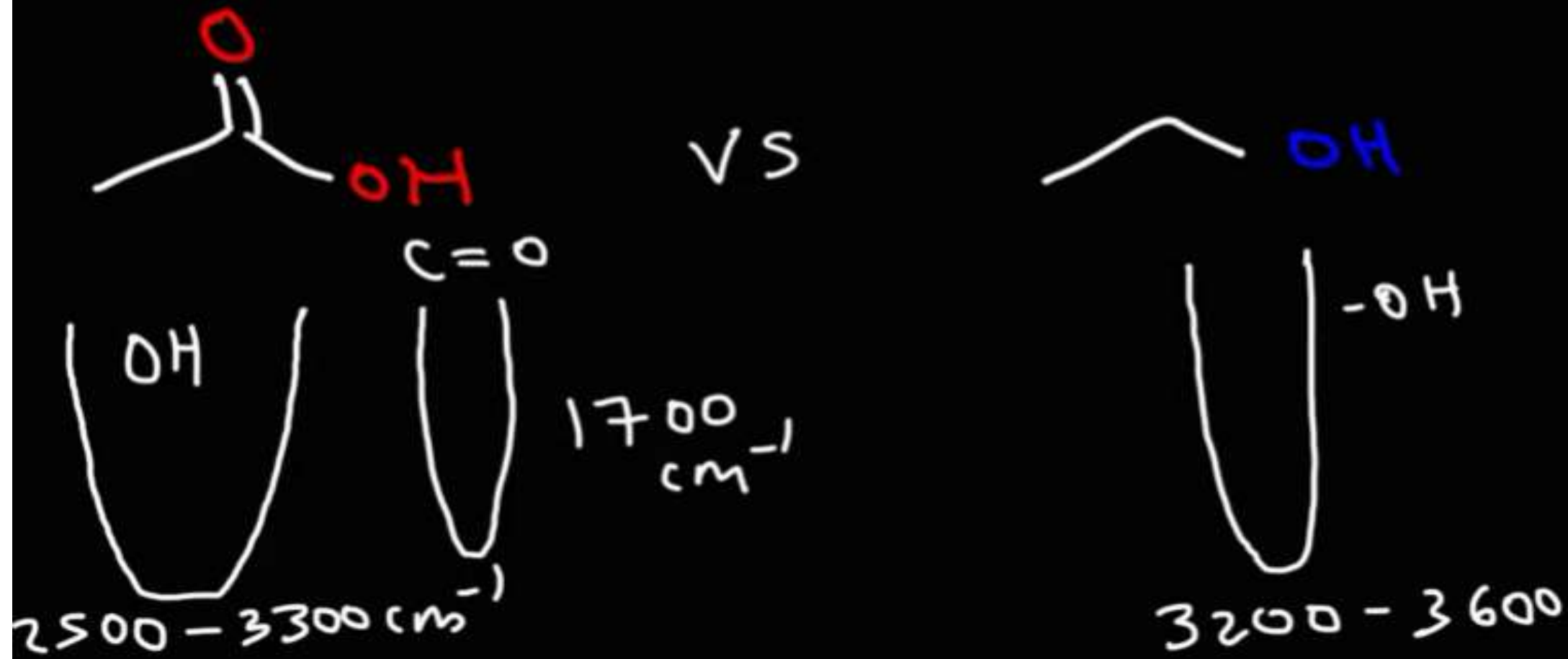


IR Spectroscopy



Aldehyde

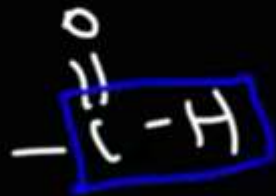


C=O



1700 cm⁻¹

vs



2900 cm⁻¹
-C-H

2700 cm⁻¹

Ketone

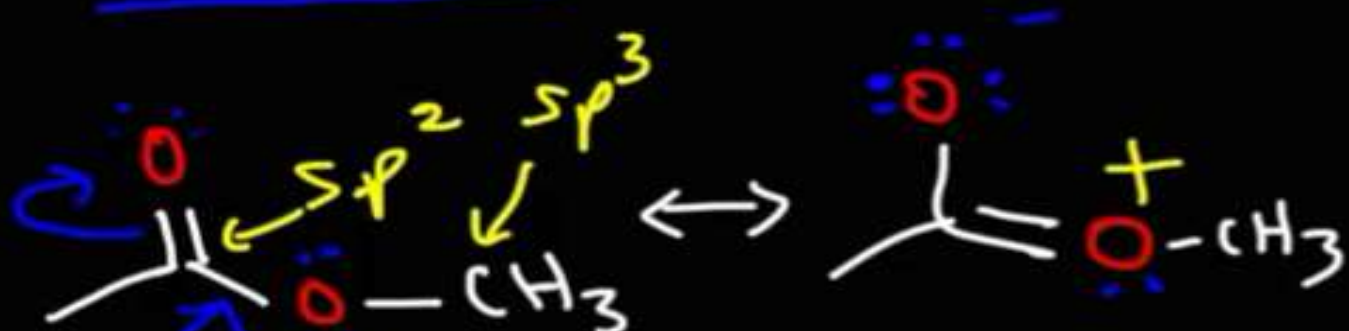


C=O



1700 cm⁻¹

Ester



C=O

C-O

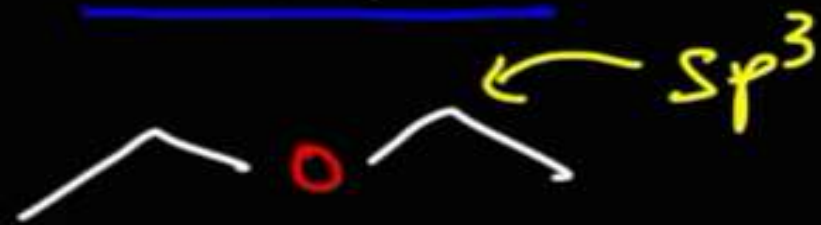
1200 - 1300 cm^{-1}

C-O

1000 - 1150 cm^{-1}

1700 cm^{-1}

Ether



C-O

1000 - 1150 cm^{-1}

Amine



W 3300 - 3500



V 3300 - 3500

Amide



C=O

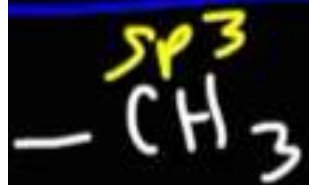


W

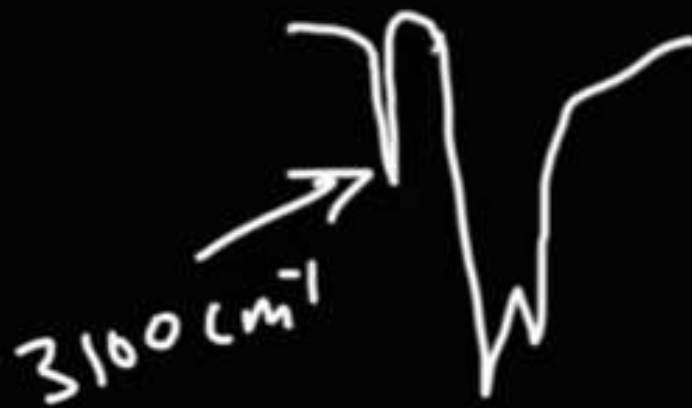
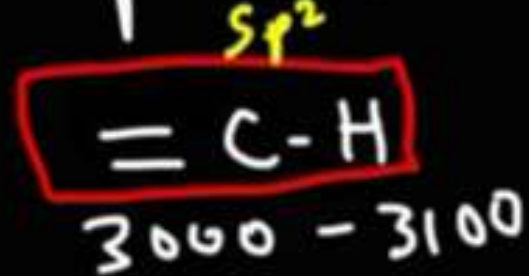
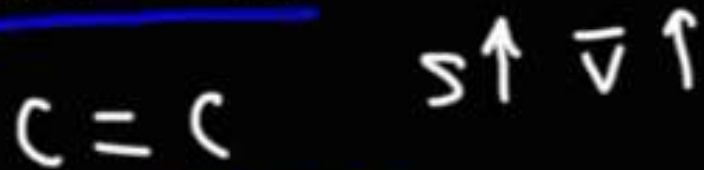
3300 - 3500

1700 cm⁻¹

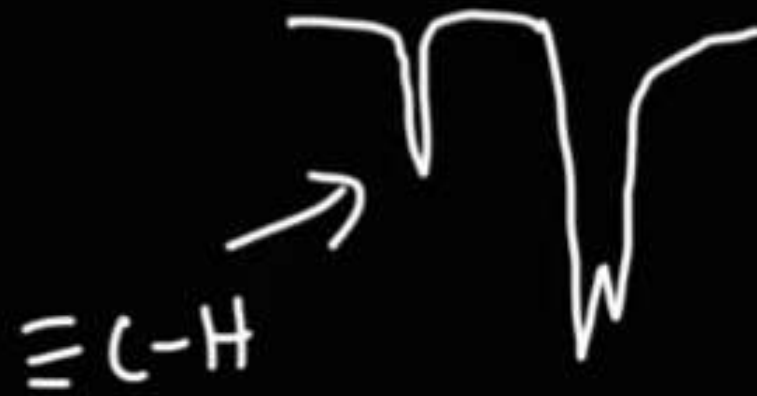
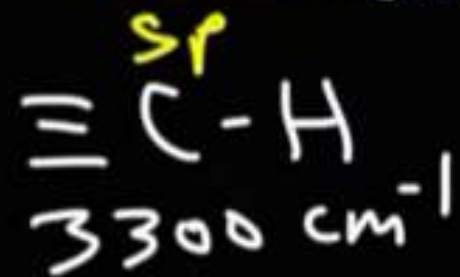
Alkane



Alkene



Alkyne



mass ↑

$\bar{\nu}$ ↓



2900 cm^{-1}



2100



1000 - 1200



600 - 800



500 - 600

Bond strength ↑

$\sqrt{\text{V}}$ ↑

C - C 1000 - 1200

C = C 1660

C ≡ C 2200

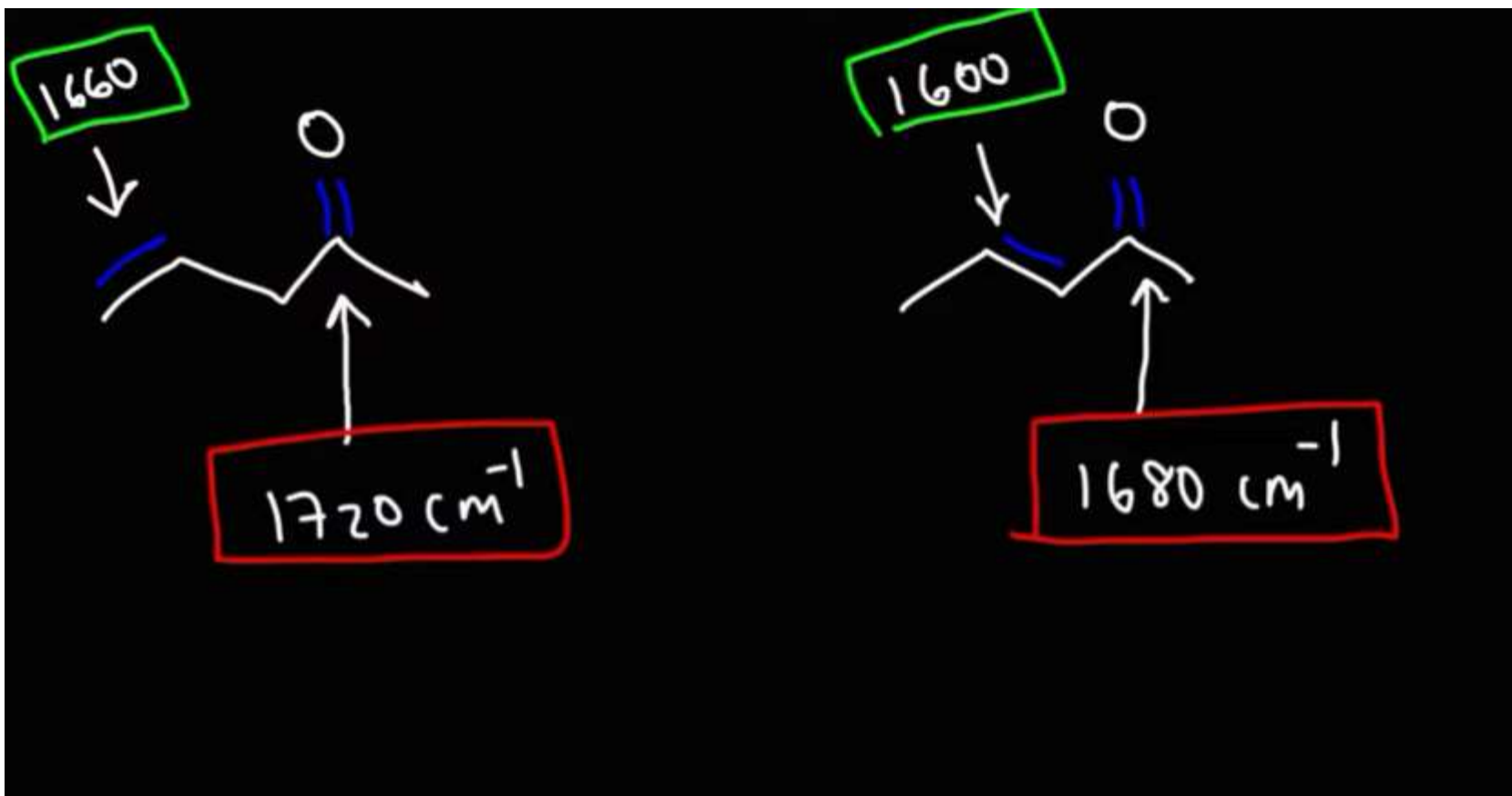
C - O 1000 - 1300

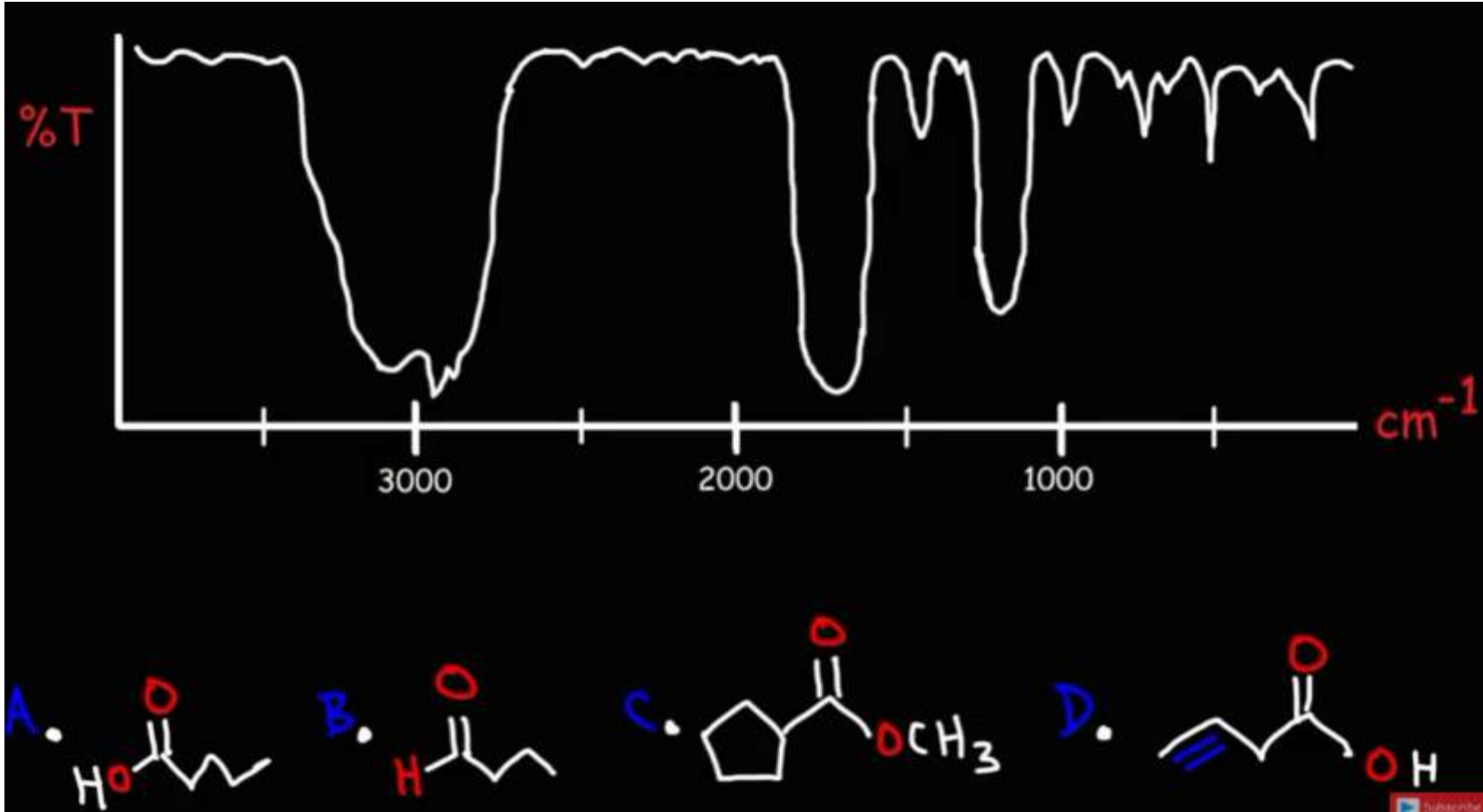
C = O 1700

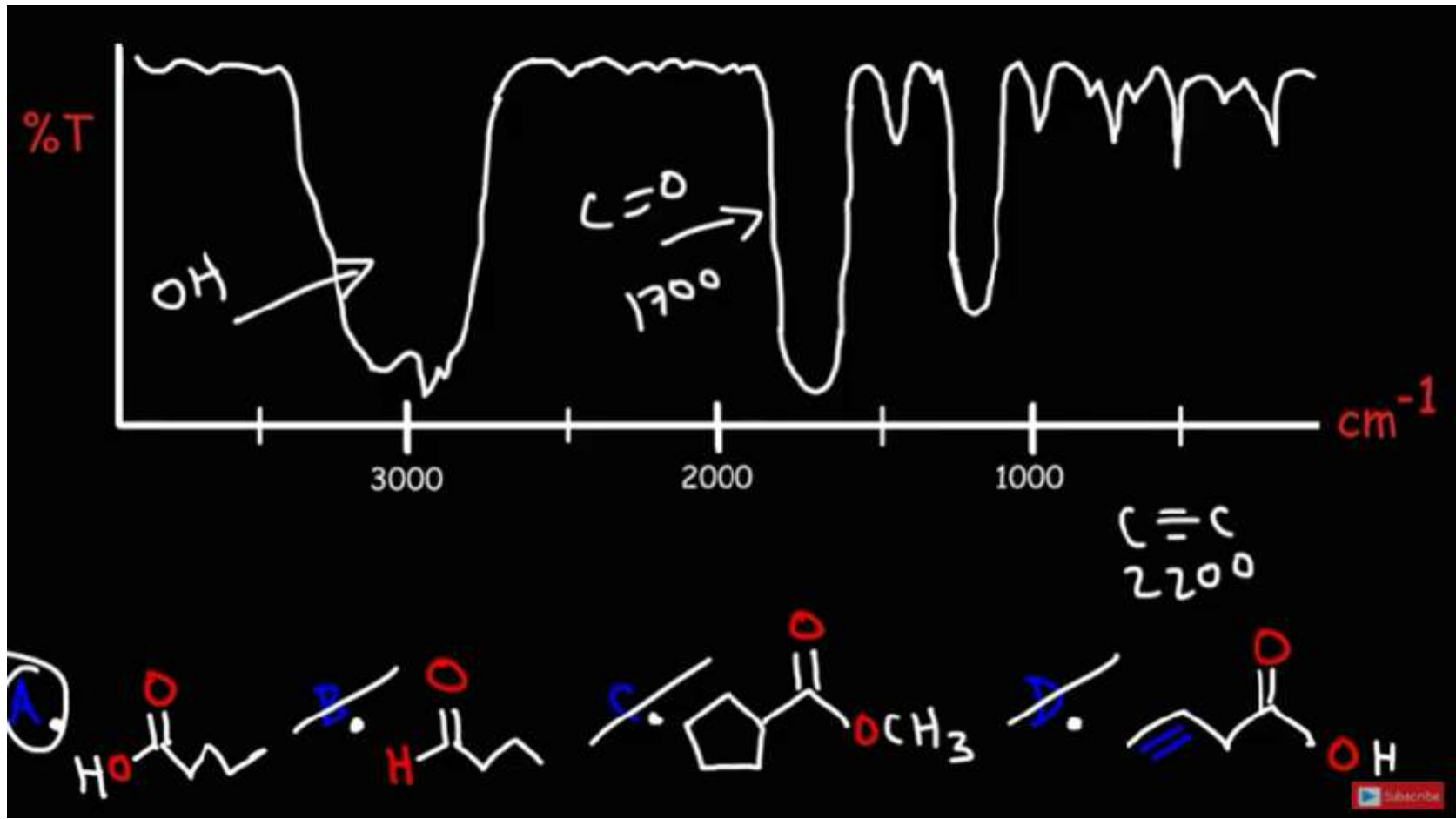
C - N 1000 - 1200

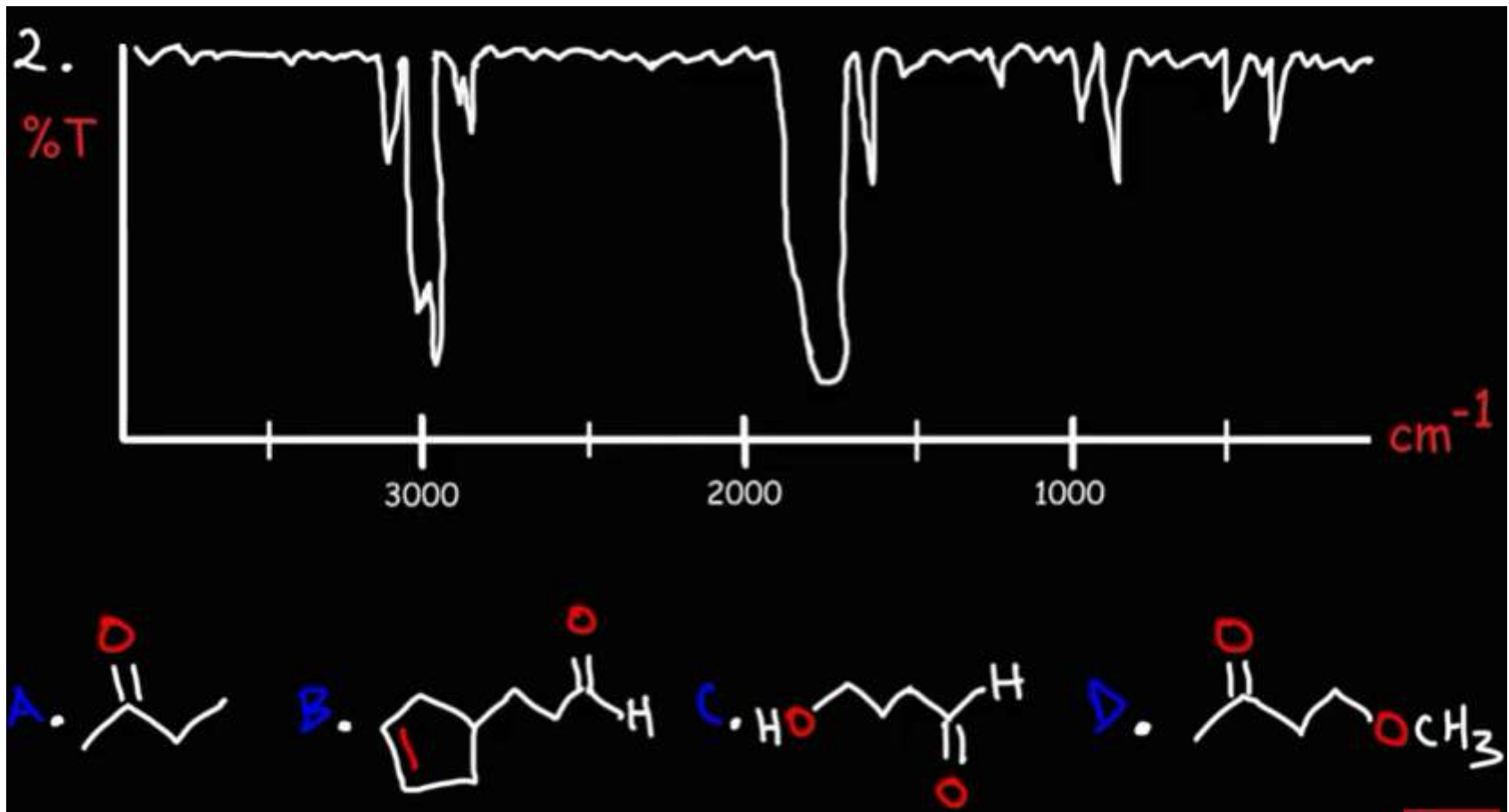
C = N 1650

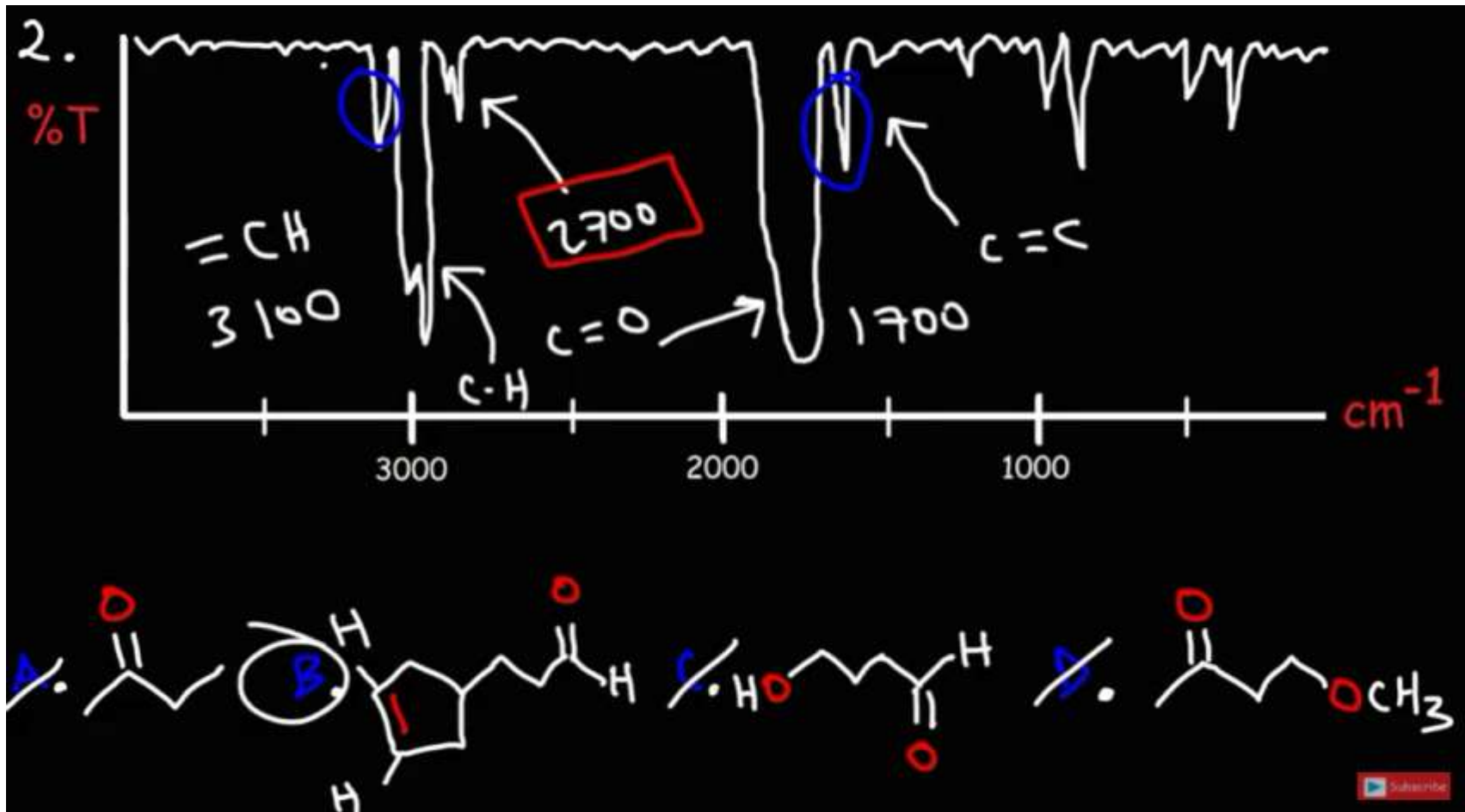
C ≡ N 2200

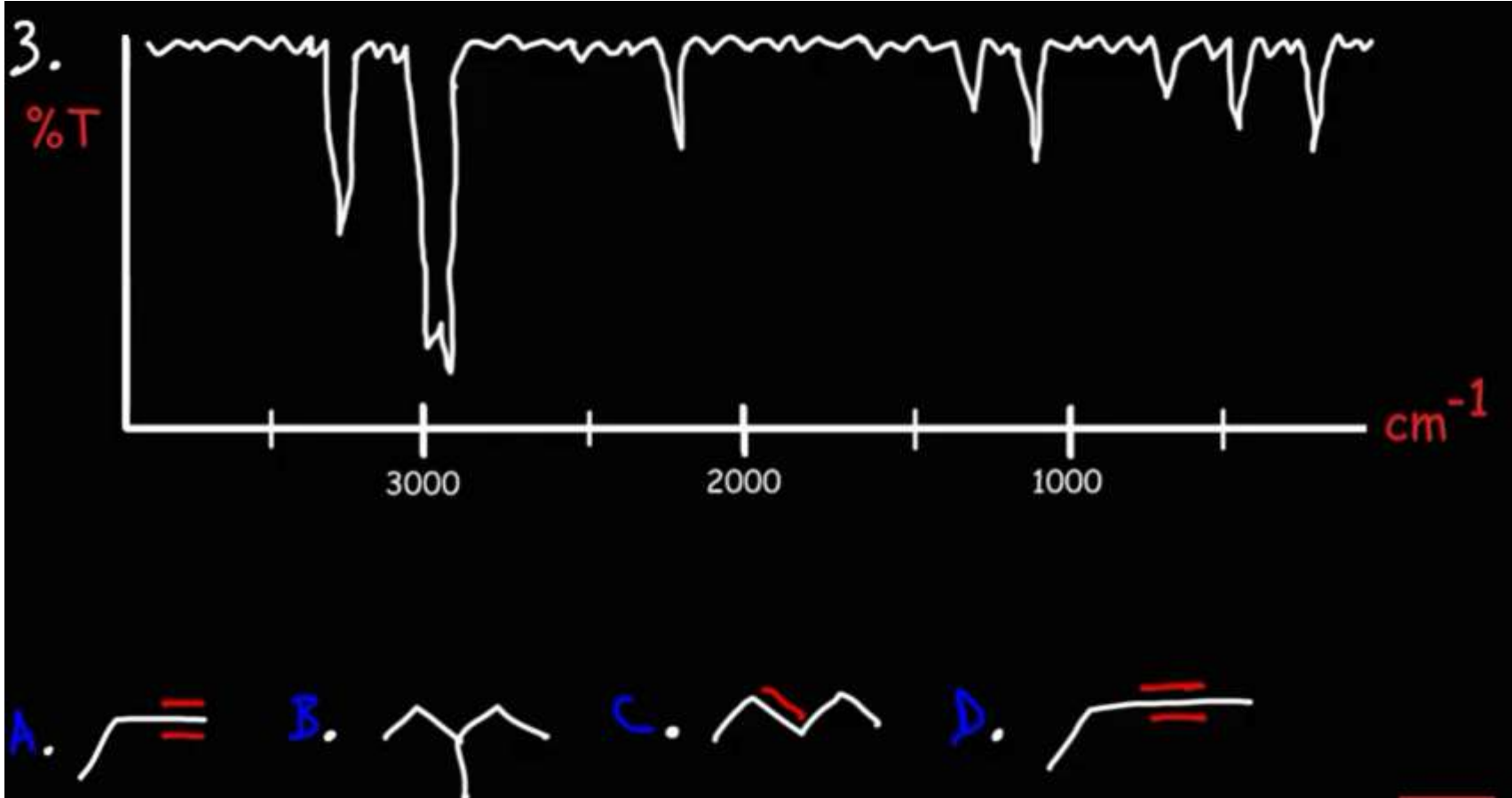


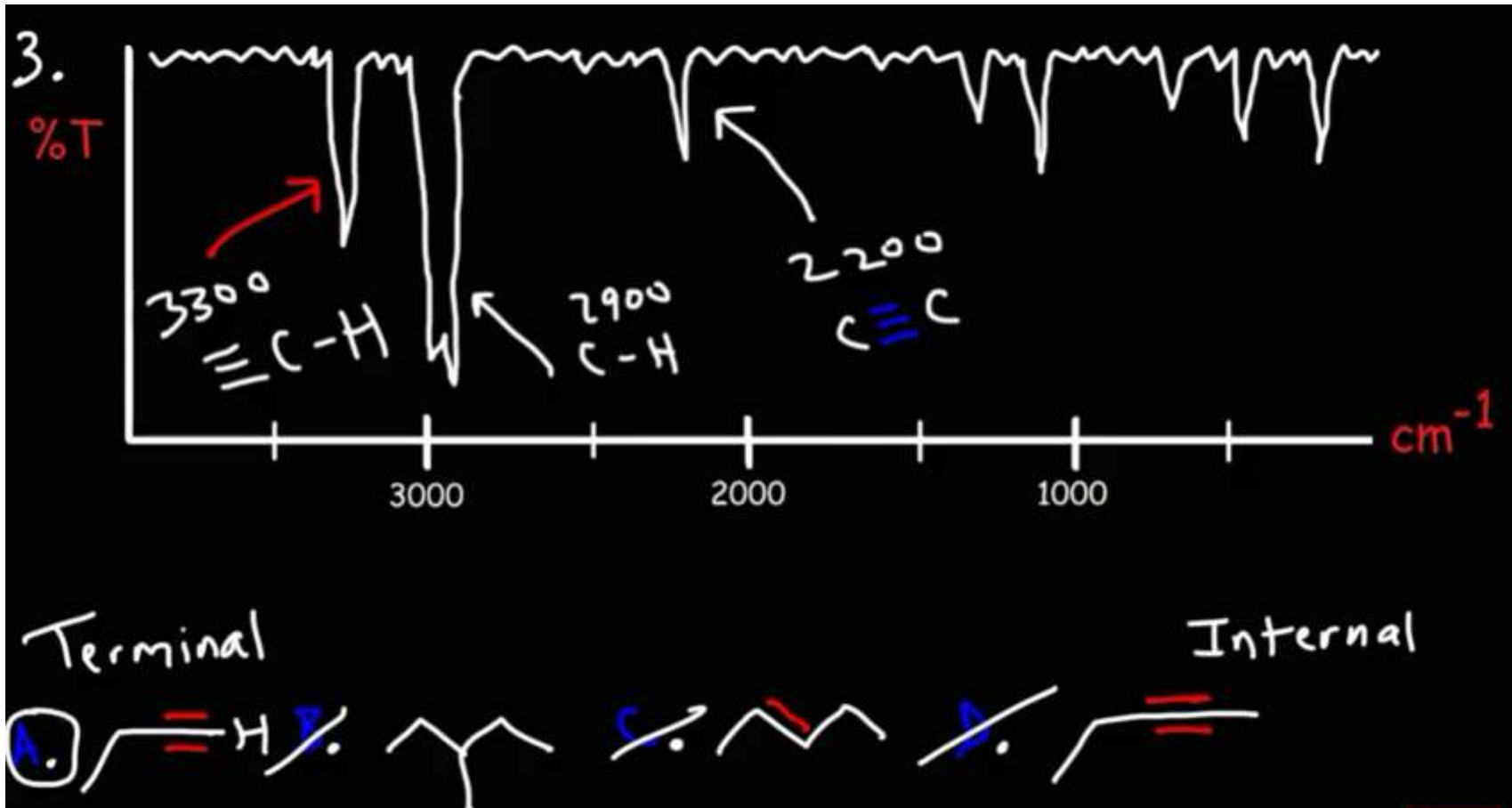


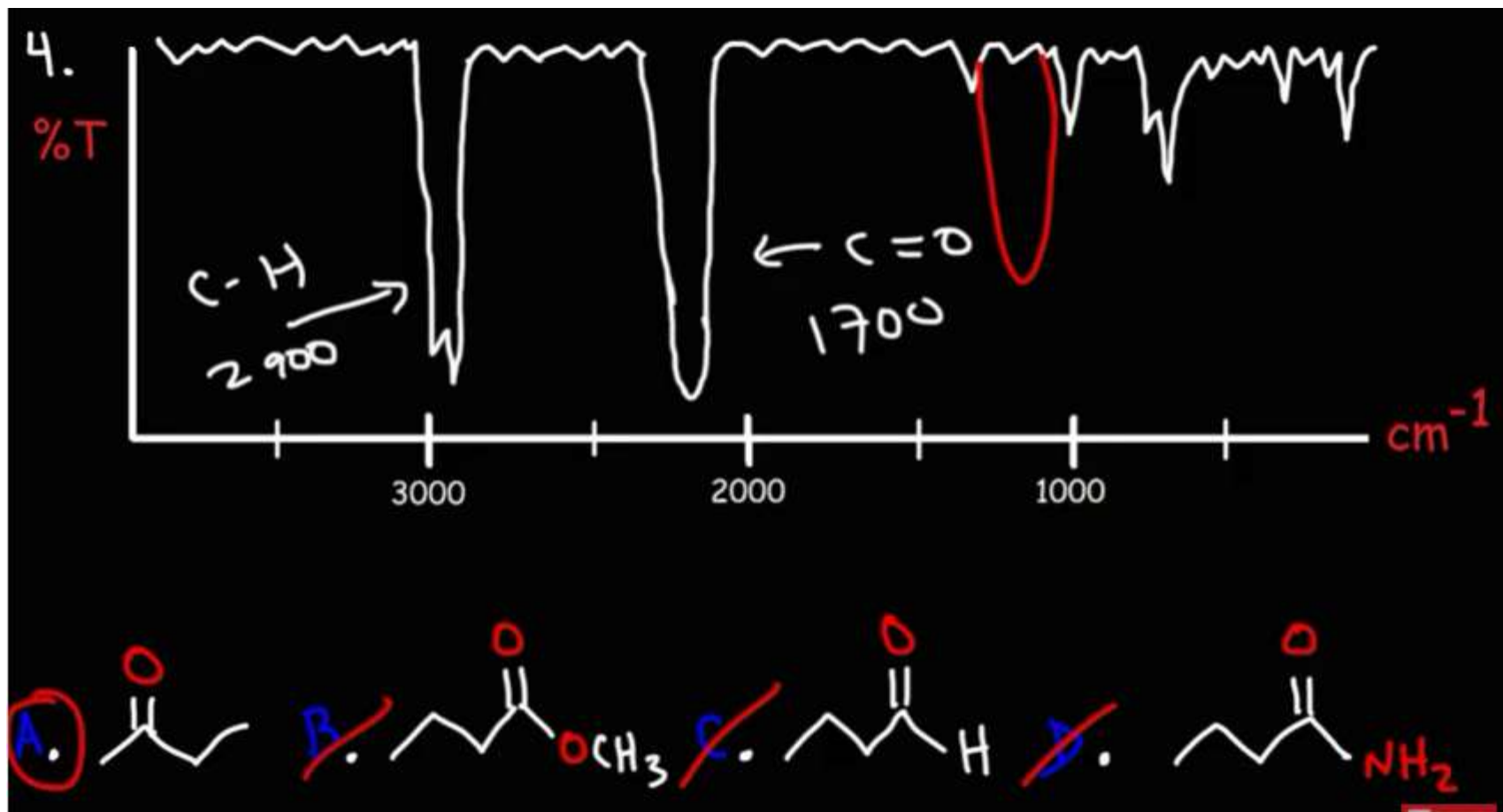


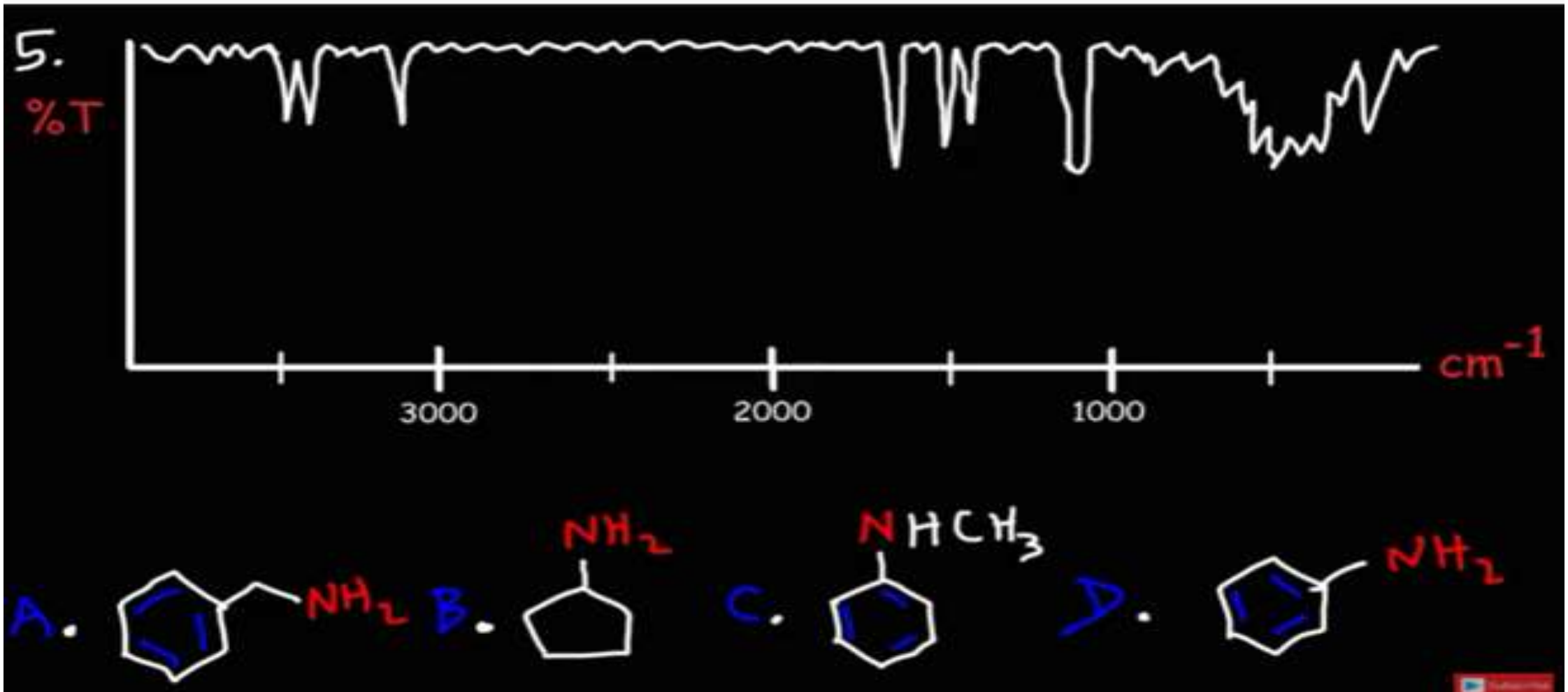


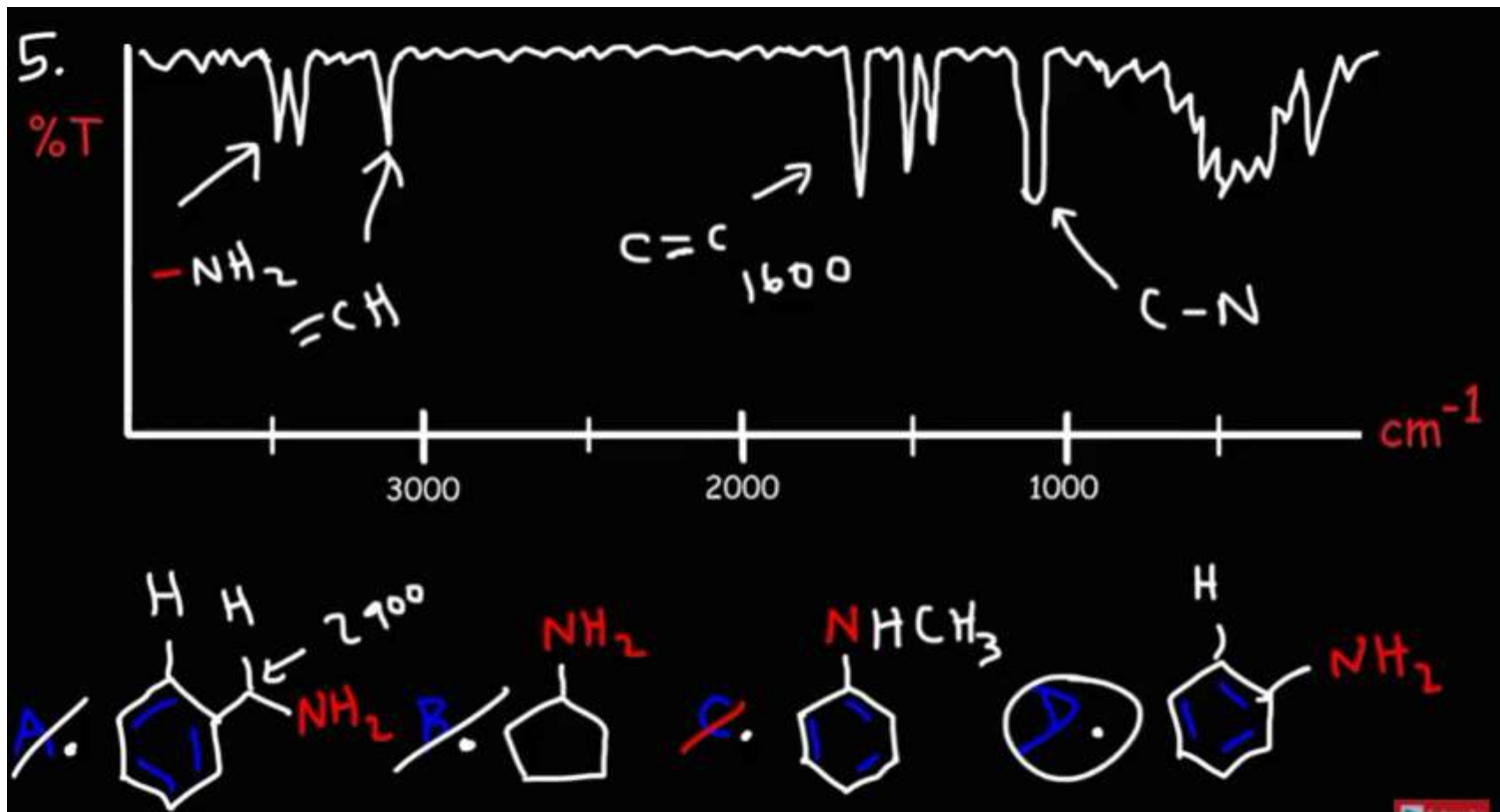


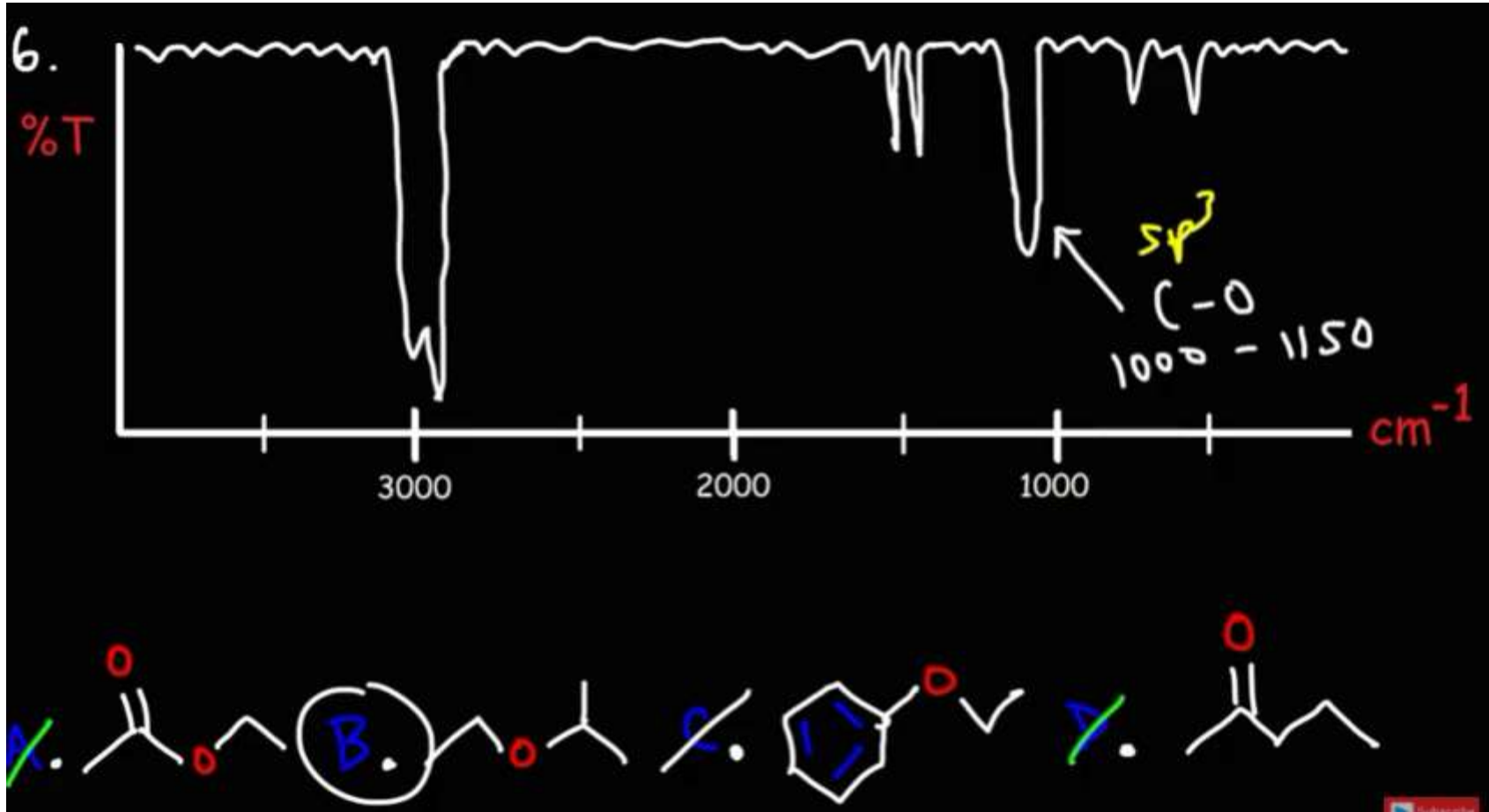






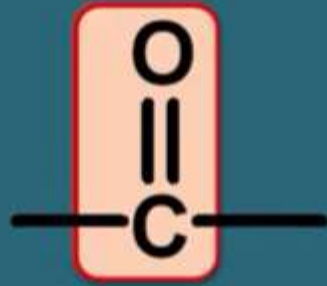






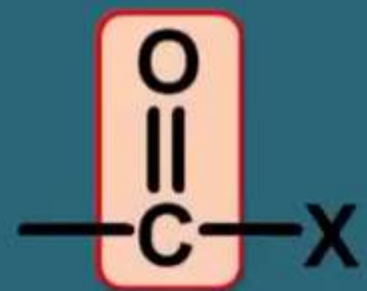
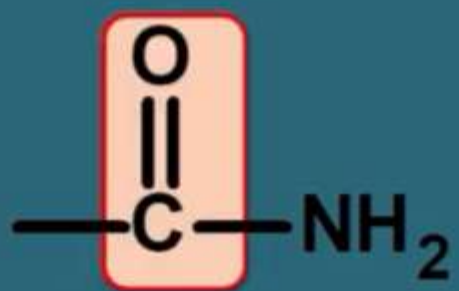
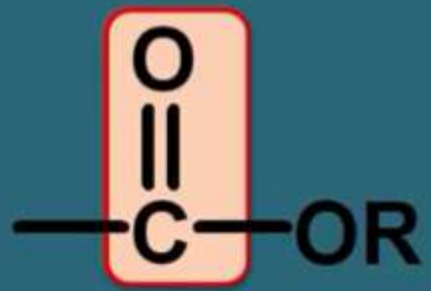
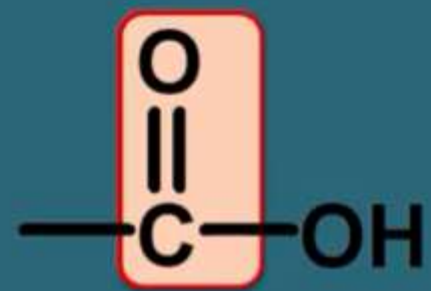
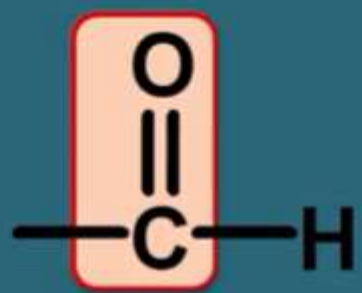
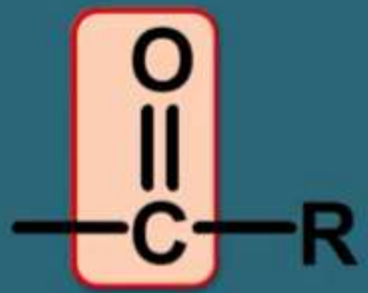
Interpretation in IR spectroscopy

Carbonyl group

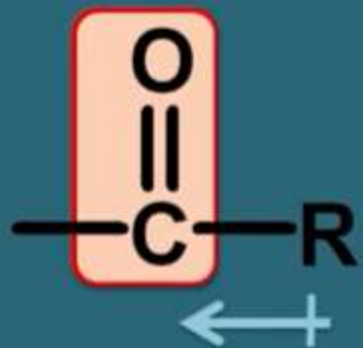


1700-1800cm⁻¹

1. Strong peak
2. Present in many functional groups
3. Can be differentiated easily



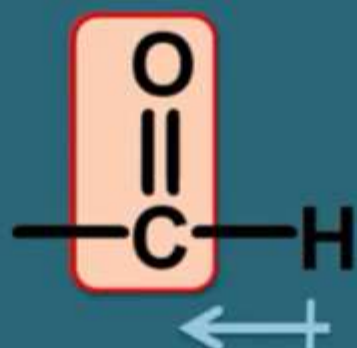
1



Ketones

1710 cm⁻¹

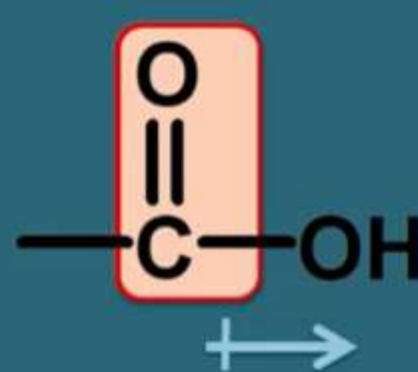
2



Aldehydes

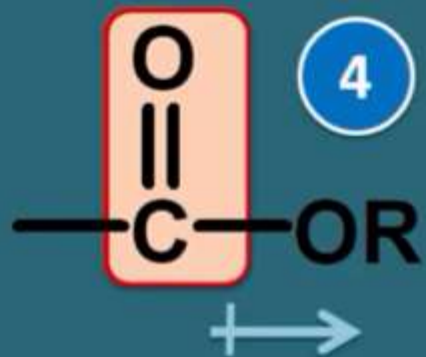
1720 cm⁻¹

3

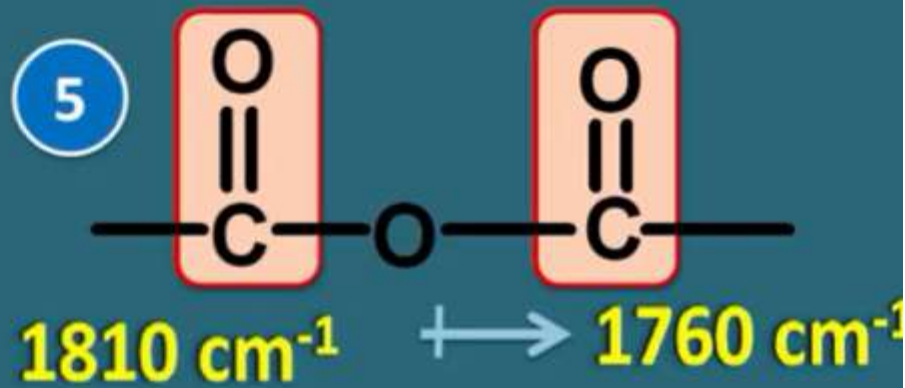


Acids

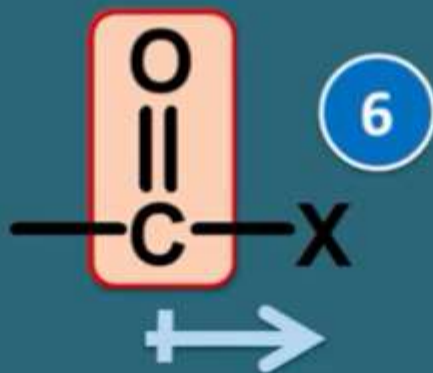
1730 cm⁻¹



Esters
 1750 cm^{-1}

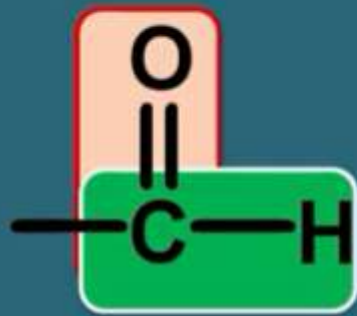


Anhydrides



Acid halides
 1800 cm^{-1}

Aldehydes vs Ketones

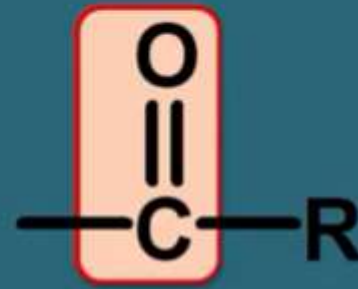


$\text{C}=\text{O}$

1720 cm^{-1}

$\text{C}-\text{H}$

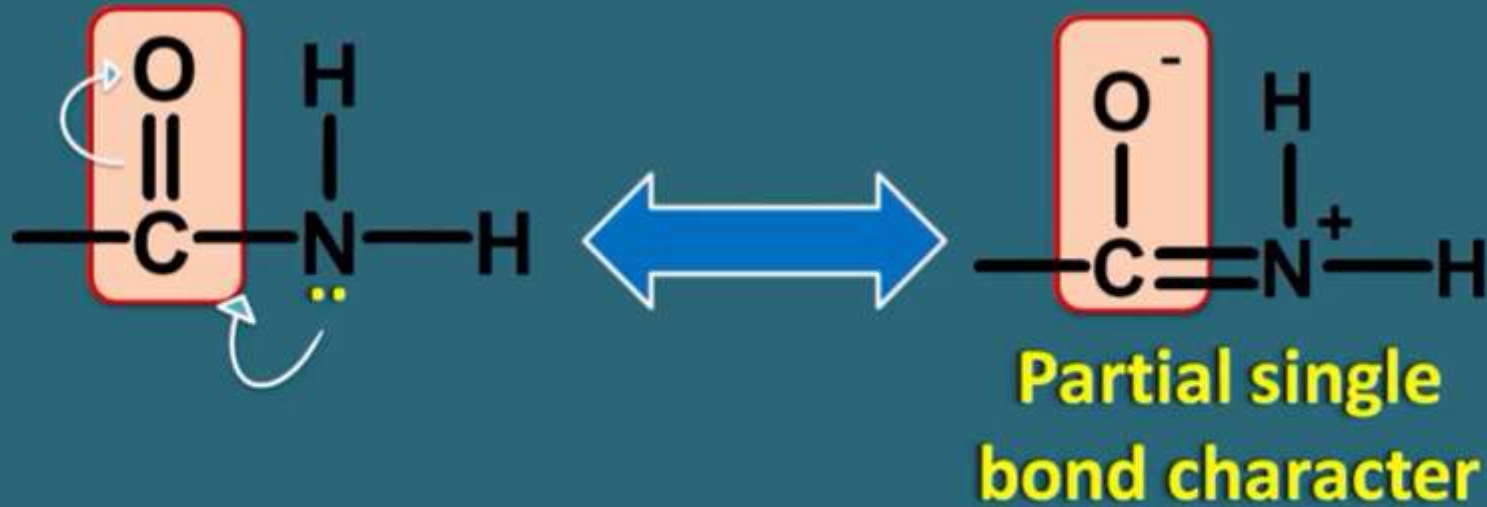
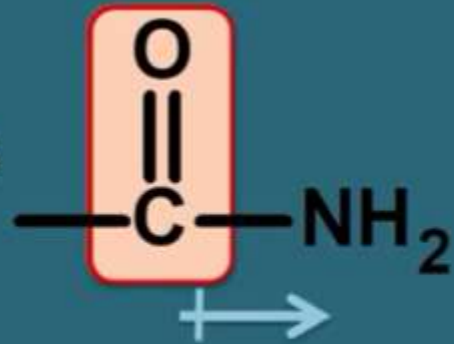
2960 cm^{-1}



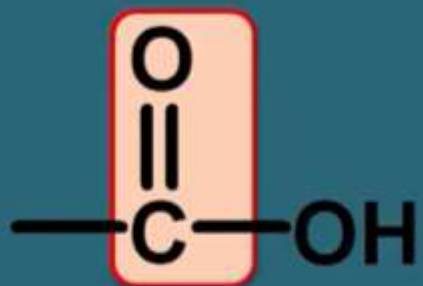
$\text{C}=\text{O}$ $1710 - 1720 \text{ cm}^{-1}$

⊗

Amides



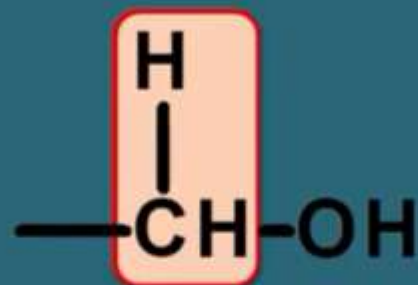
Acids vs alcohols



O-H 3600 cm^{-1}

C-O 1200 cm^{-1}

C=O 1730 cm^{-1}



O-H 3600 cm^{-1}

C-O 1100 cm^{-1}

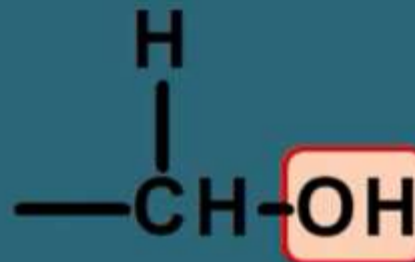


Phenols vs alcohols



O - H 3400 cm^{-1}

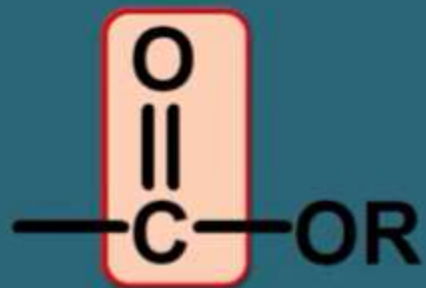
C - O 1060 cm^{-1}



O - H 3600 cm^{-1}

C - O 1100 cm^{-1}

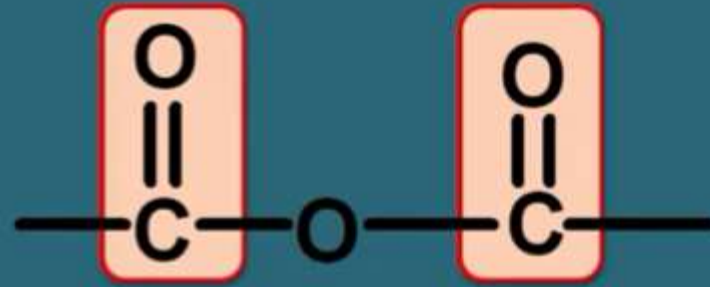
Esters



C = O **1750 cm⁻¹**

C - O **1200 cm⁻¹**

Anhydrides

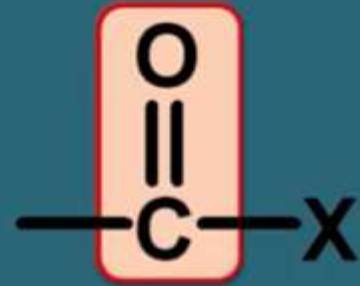


C = O 1760 cm^{-1}

1800 cm^{-1}

C - O 900 - 1300

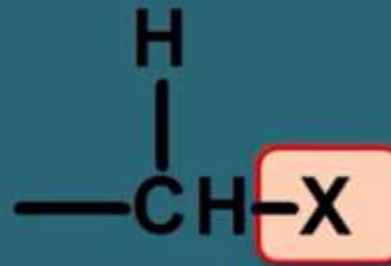
Acid chlorides



C = O **1800 cm⁻¹**

C - Cl **750 cm⁻¹**

Halides



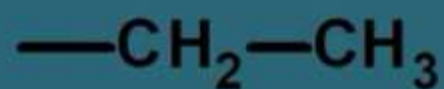
C - F **1200 cm^{-1}**

C - Br **650 cm^{-1}**

C - Cl **750 cm^{-1}**

C - I **500 cm^{-1}**

Alkyl compounds



C - H 3000 cm^{-1} =C - H 3100 cm^{-1} 3300 cm^{-1}

C - C 1200 cm^{-1} C = C 1600 cm^{-1} 2100 cm^{-1}

How IR spectroscopy works?

IR region

Wavelength

near IR

750 nm – 2.5 μm

mid IR

2.5 μm – 25 μm

4000 – 400 cm^{-1}

far IR

25 μm – 0.1 mm

Hooke's law



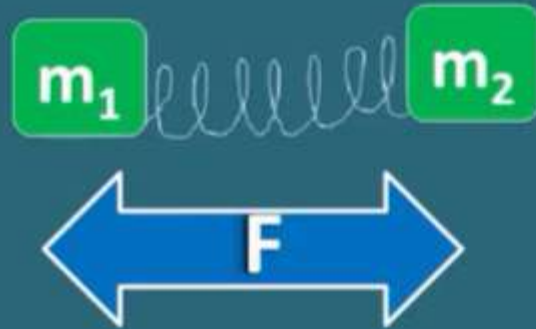
$K =$ force constant

$$F \propto x$$

$$F = -kx$$

$$v = \frac{1}{2\pi} \sqrt{\frac{k}{m_1}}$$

Hooke's law



K = force constant

μ = reduced mass

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

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

Hooke's law in IR spectra



IR

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

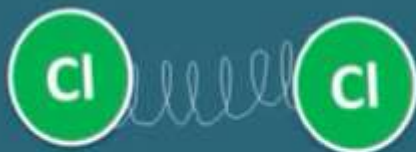
$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

Vibrational transitions

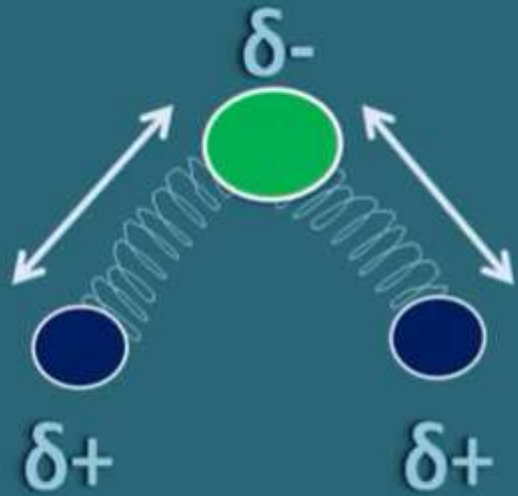
Stretching

Bending

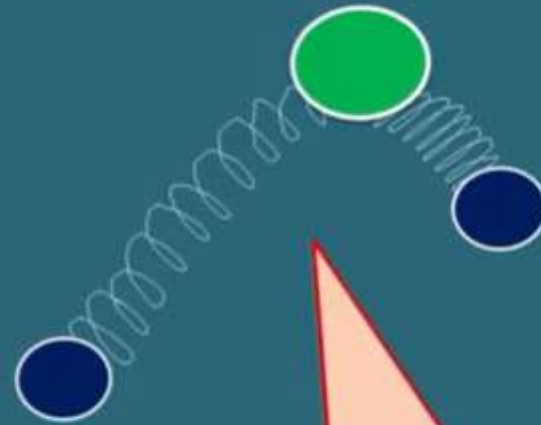
All transitions are not IR active



What is required for IR absorption?



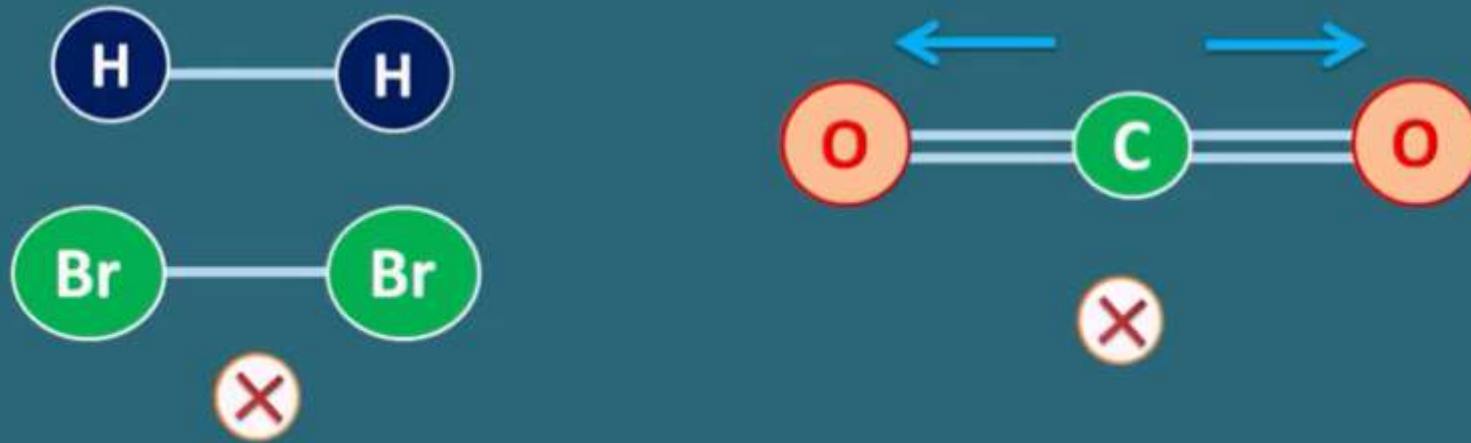
$$\mu = q \times d$$



Change in dipole moment

Which types of molecules show IR absorption?

Net change in the dipole moment



Which types of molecules show IR absorption?

O-H

C-C

C=O

N-H

C=C

C-Cl

C-H

C≡C

C-Br

Frequency of IR absorption

1. Force constant
2. Reduced mass

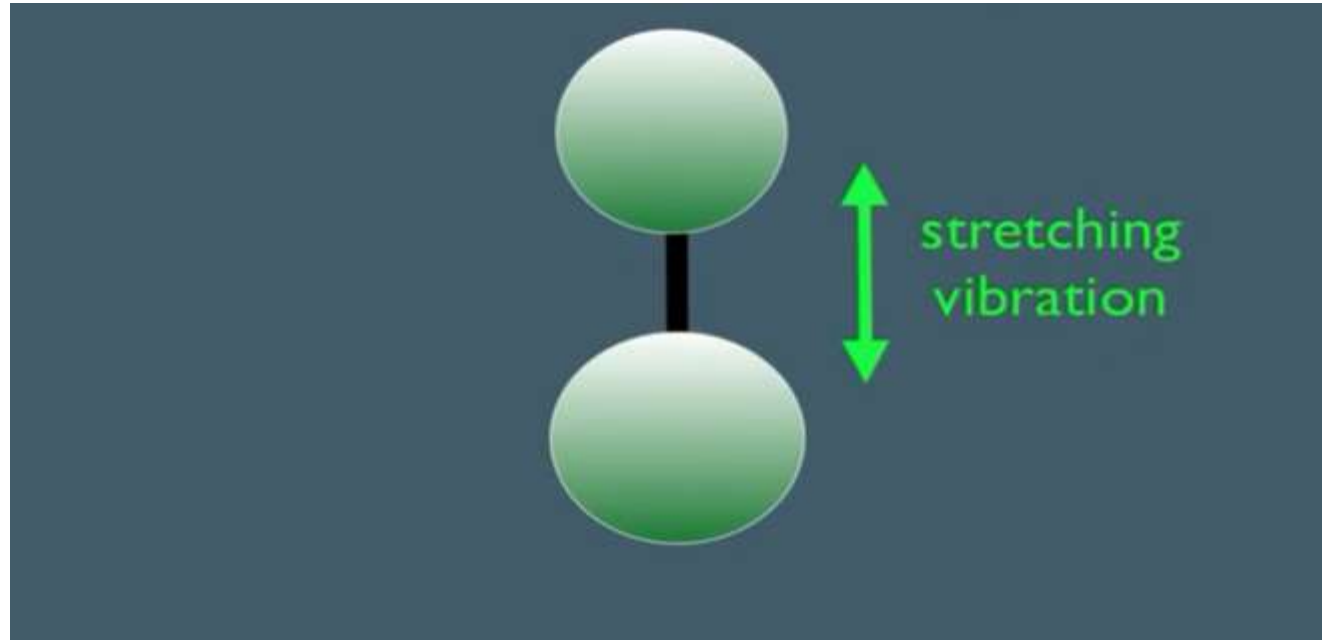
$$\nu = c/\lambda = c\bar{\nu}$$

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

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

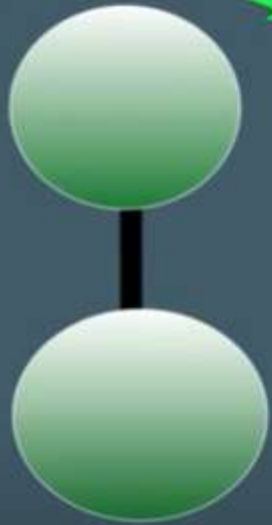
Key Points

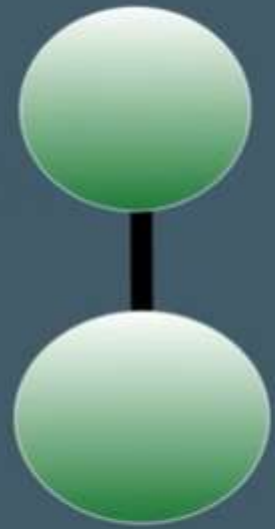
1. Different functional groups bend, stretch, and wag at different frequencies
2. A functional group will absorb light if the frequency of the light matches the frequency of stretching, bending, or wagging
3. IR spectra show absorption bands that enable to determine if certain functional groups are present in a molecule



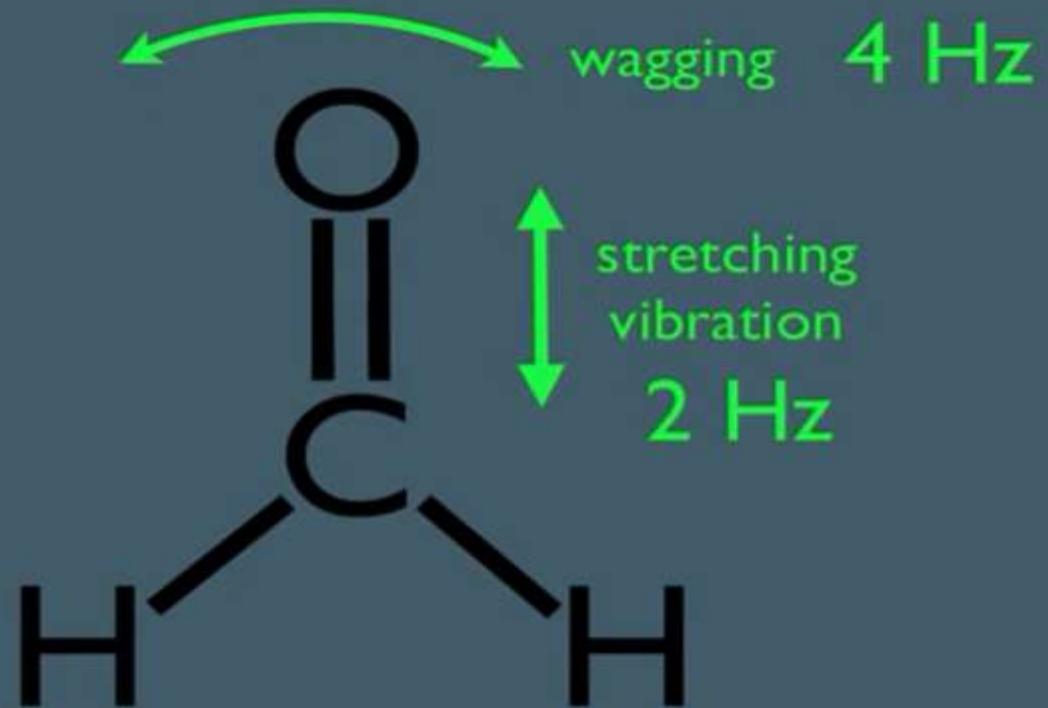


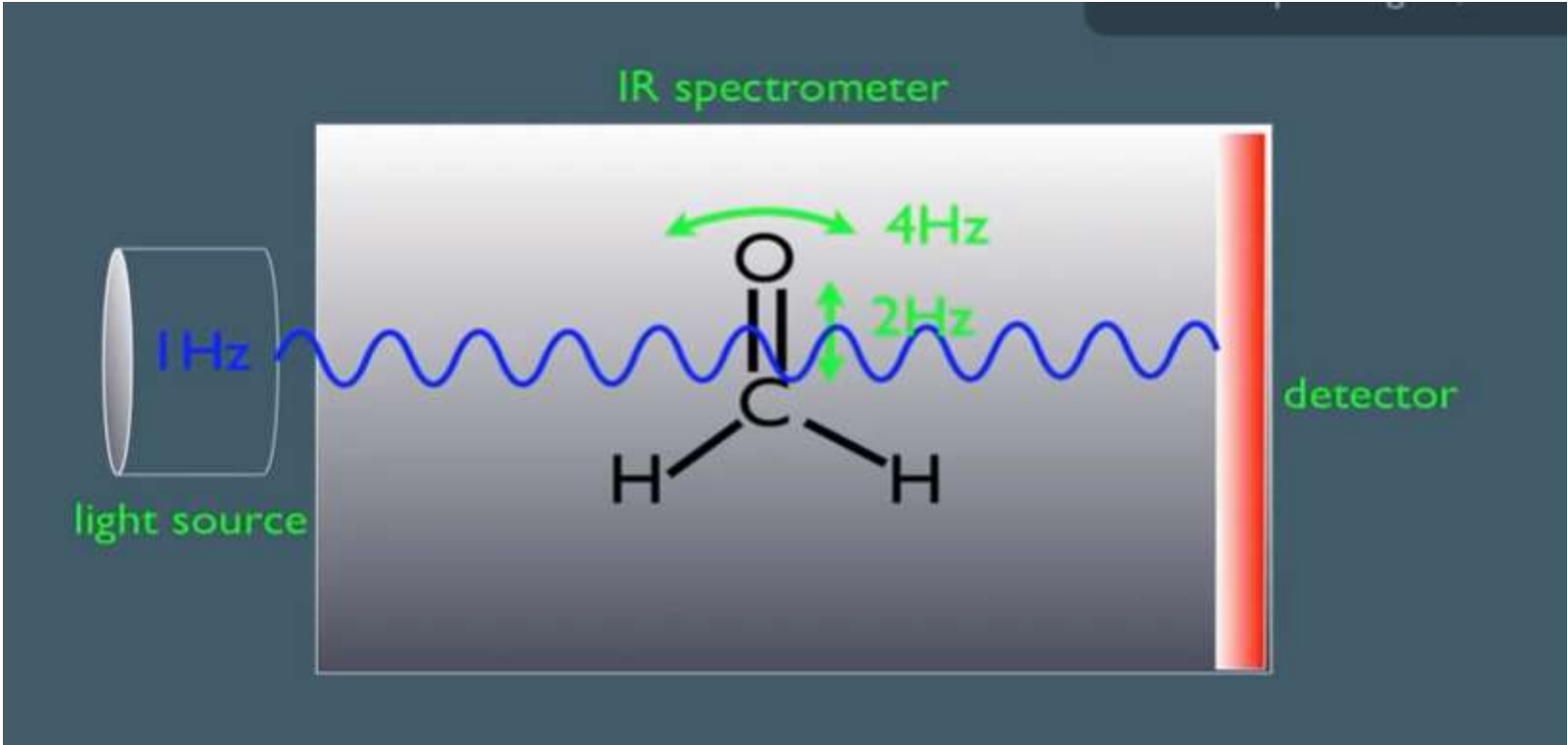
wagging

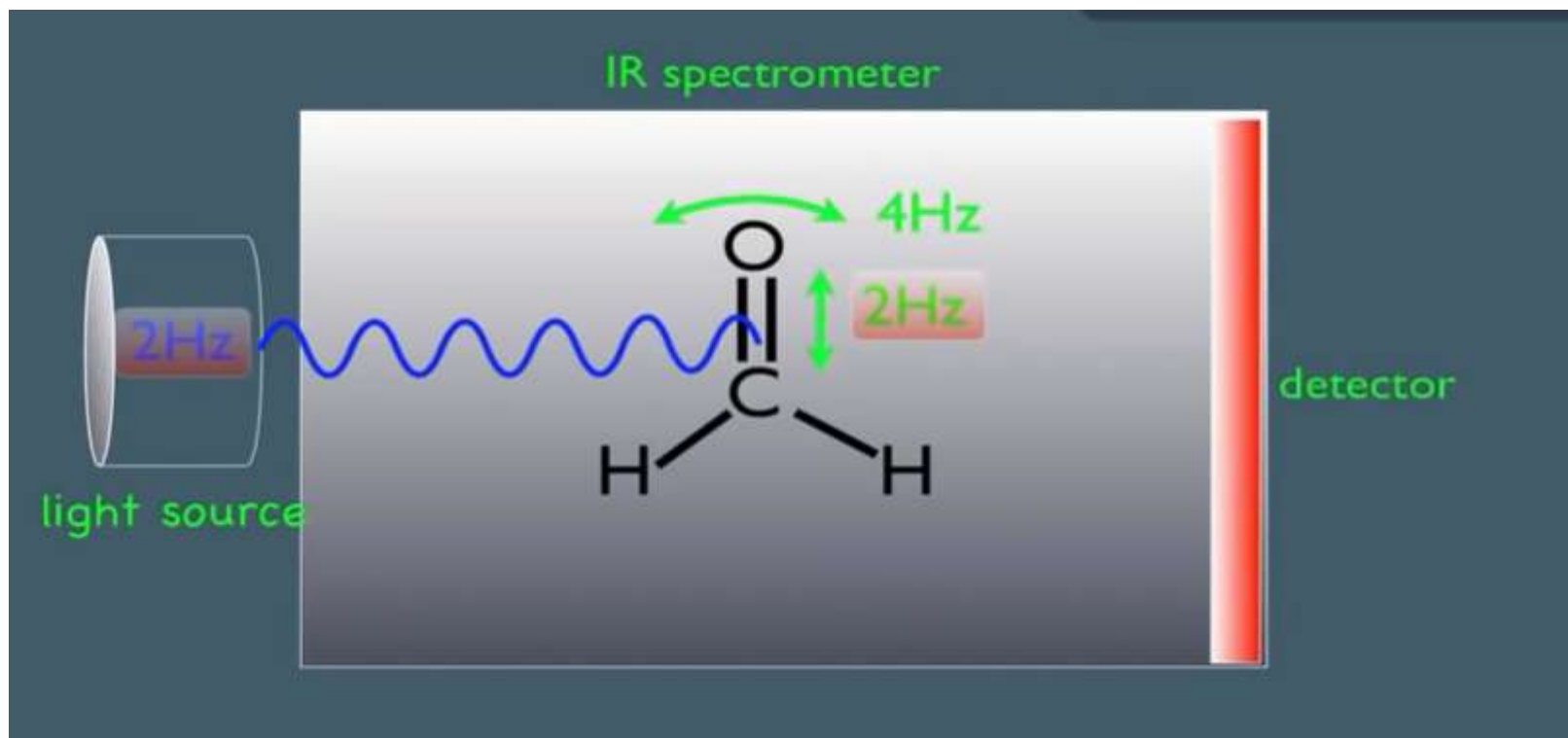


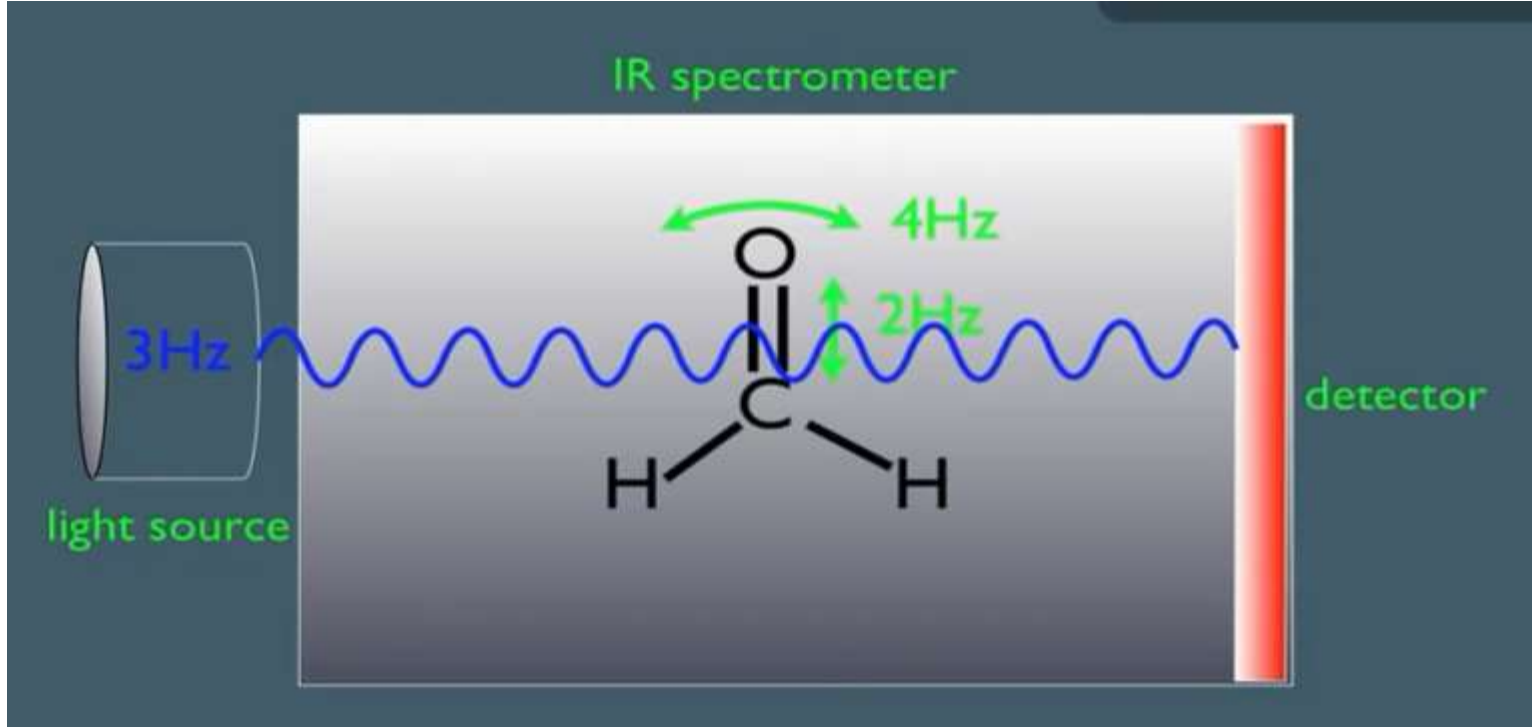


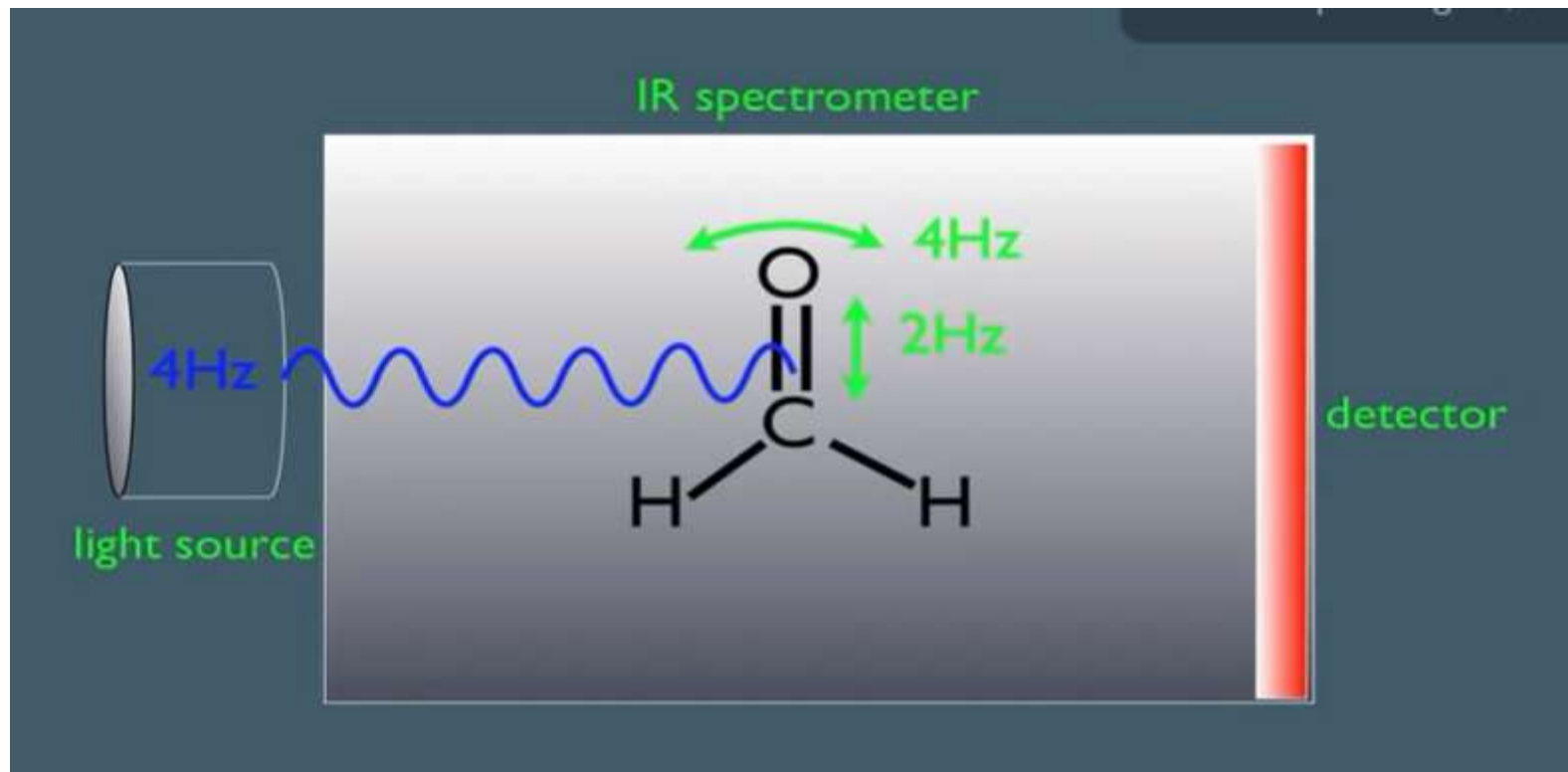
stretching
vibration
2 Hz

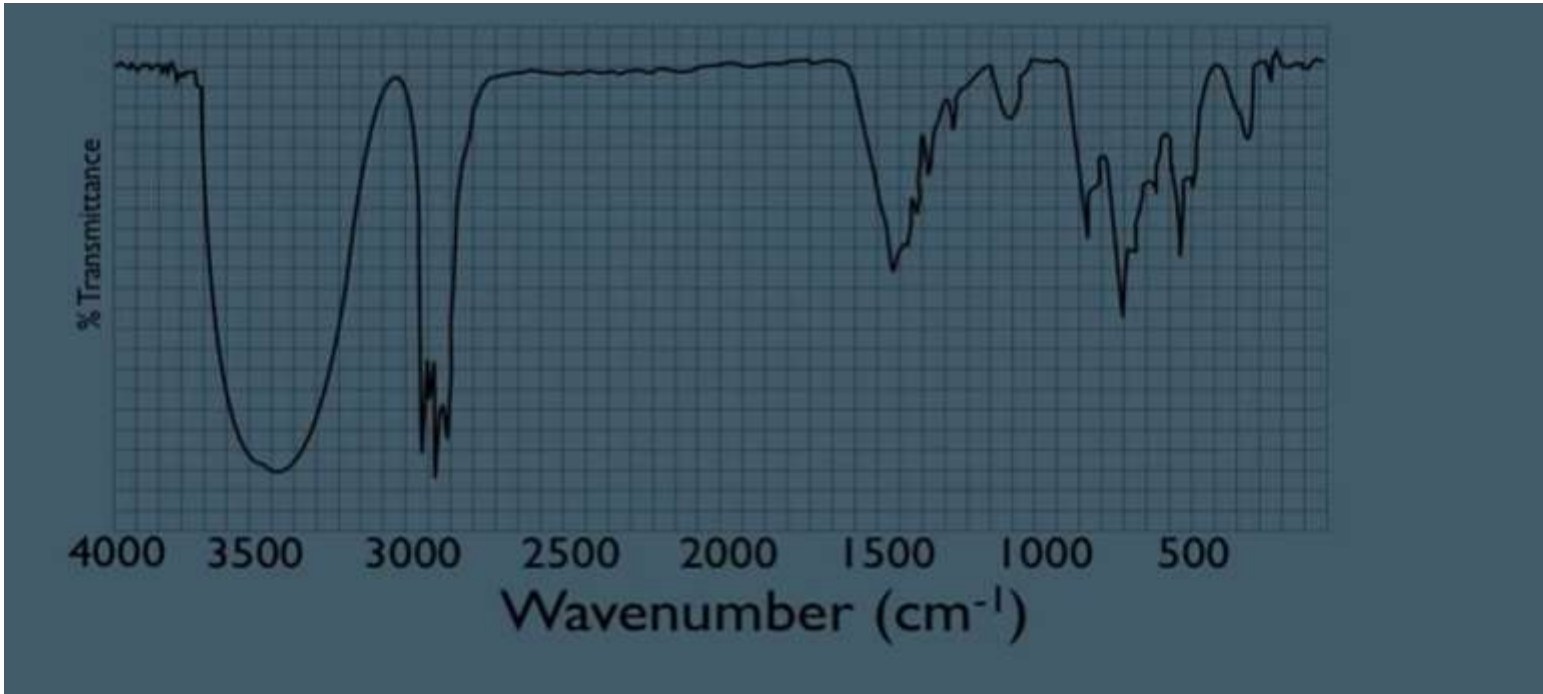


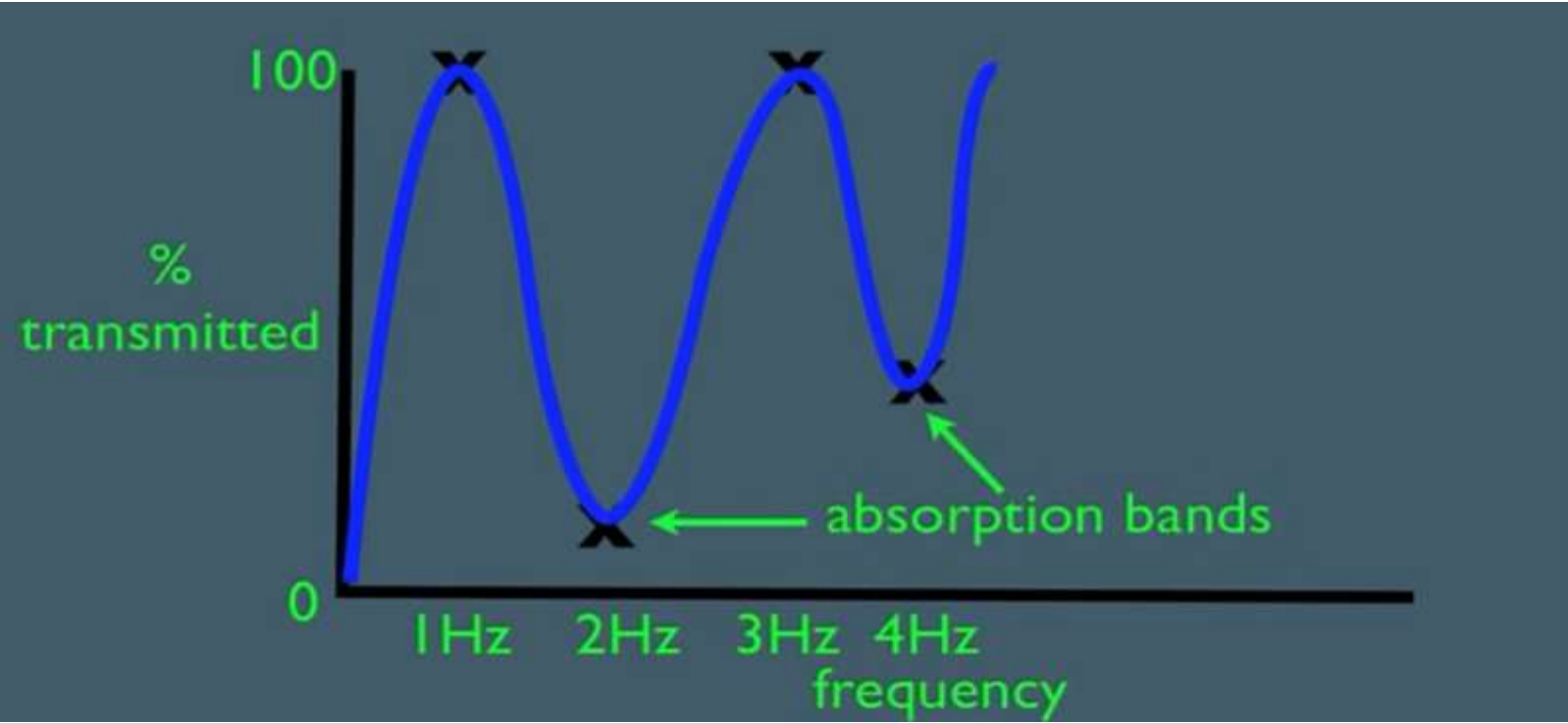


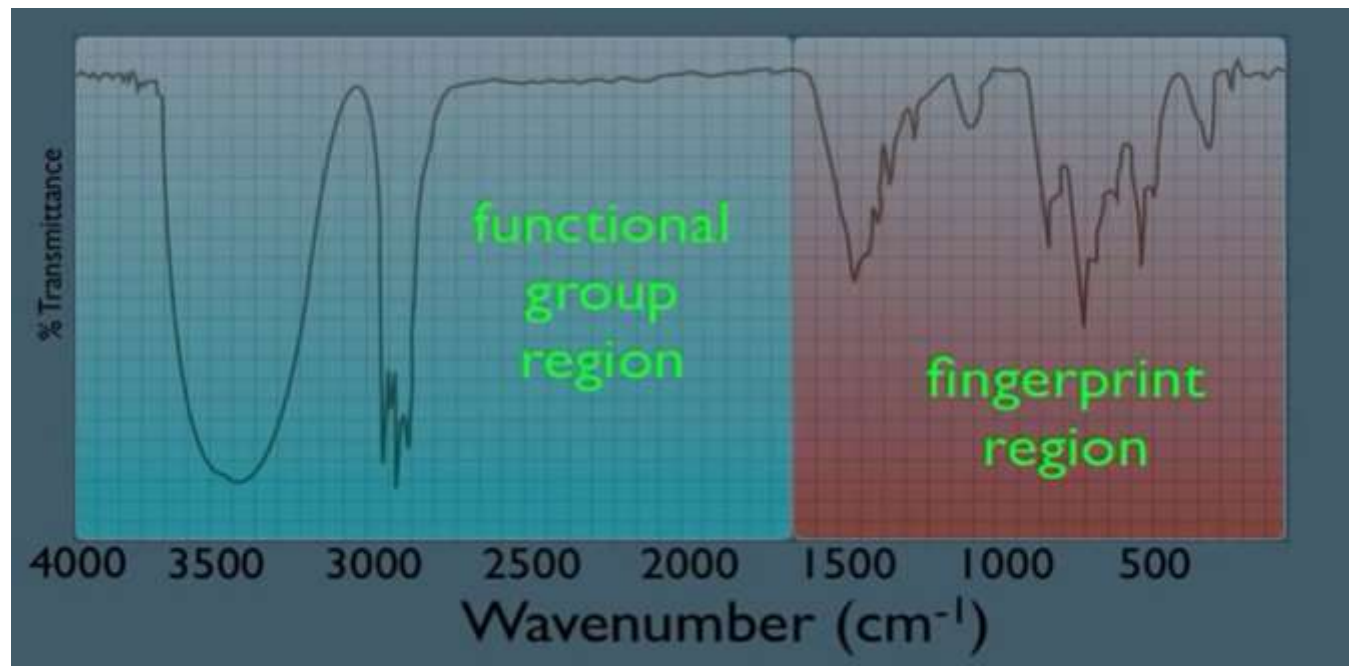






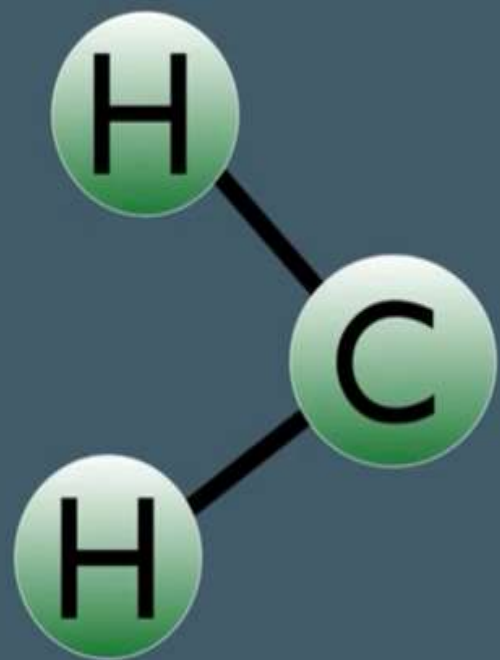




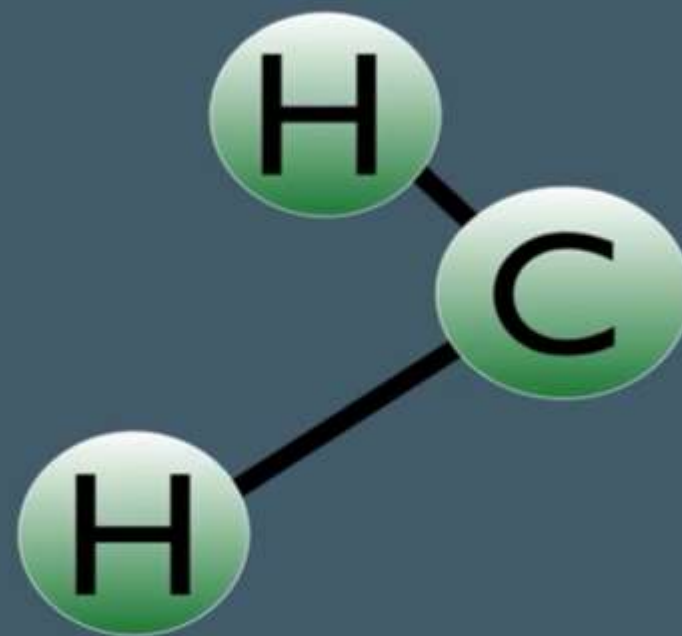


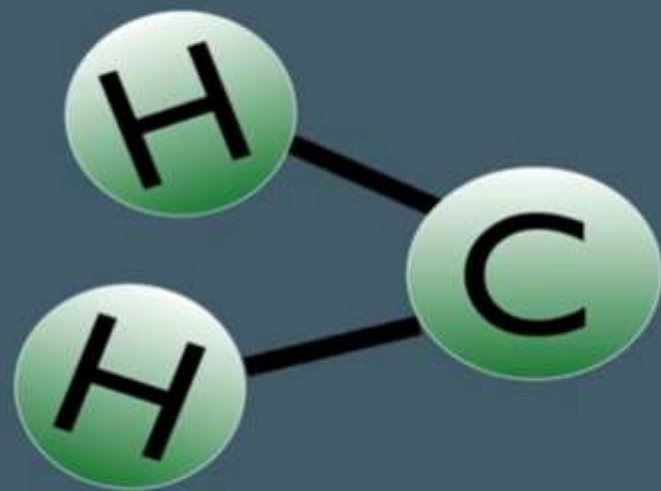
functional group wavenumbers

bond	wave#	intensity
O—H	3650-3200	strong, broad
C—H	3300-2700	medium
N—H	3500-3300	medium, broad
C≡N	2260-2220	medium
C≡C	2260-2100	weak-medium
C=C	1680-1600	medium
C=N	1650-1550	medium
C=O	1780-1650	strong
C—O	1250-1050	strong

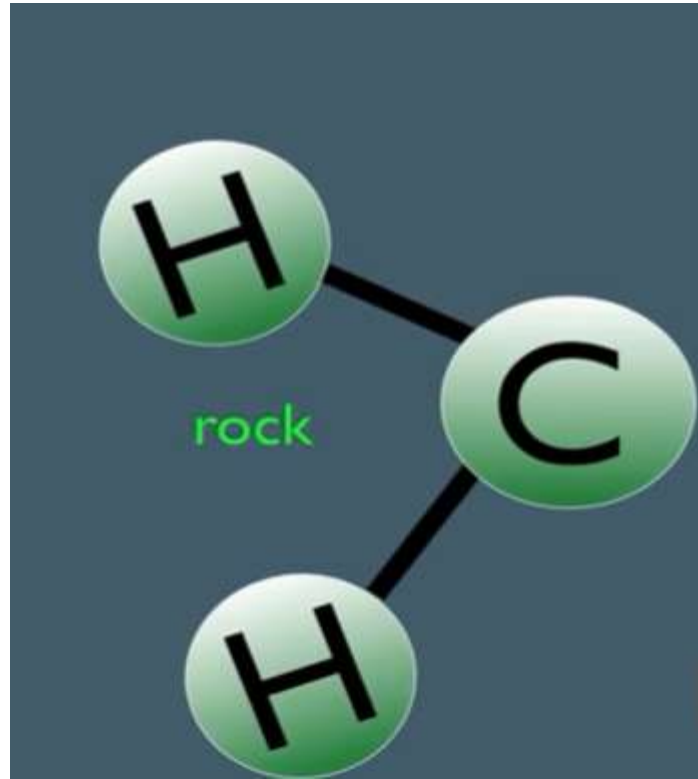


symmetrical
stretching



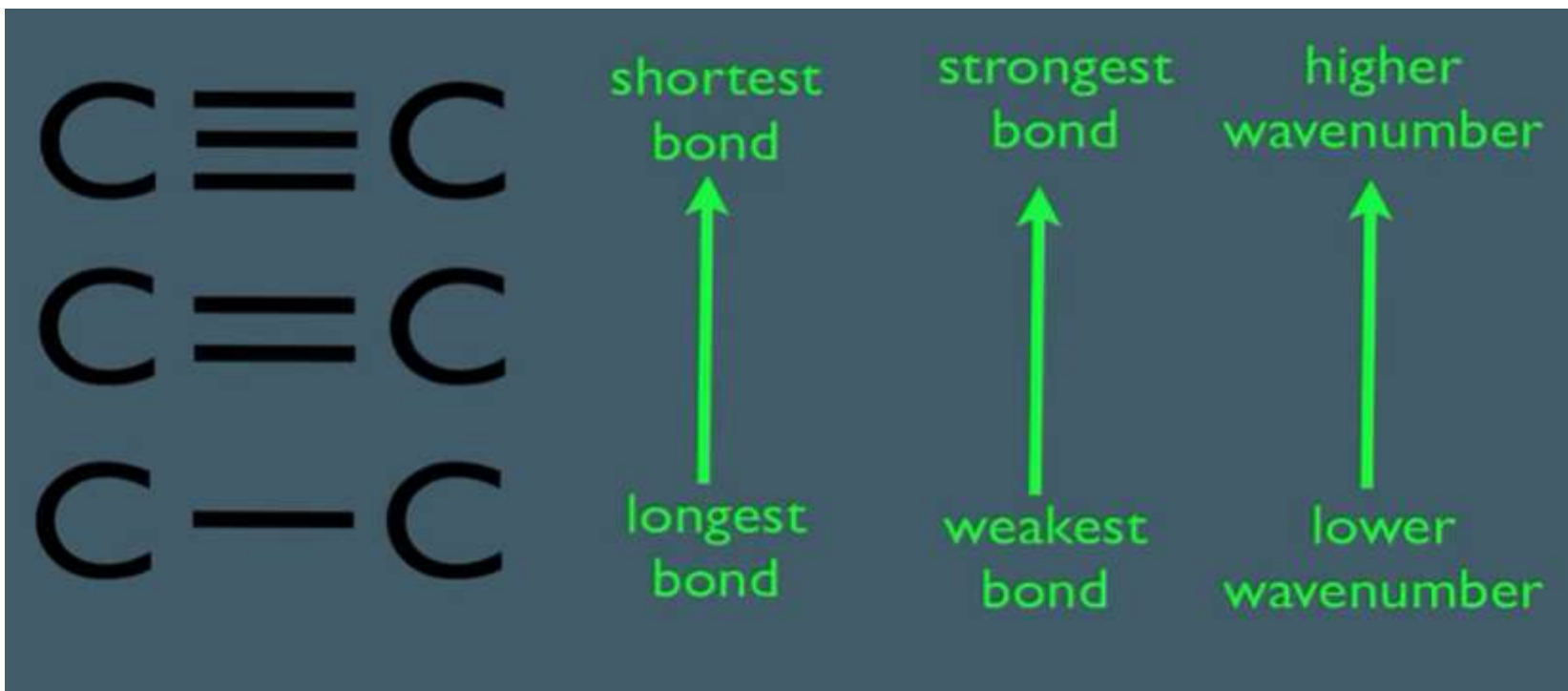


scissor



Key Points

1. The stronger the bond, the higher the frequency/wavenumber
2. The lighter the atoms, the higher the frequency/wavenumber
3. The broadening of an OH absorption band is due to hydrogen bonding
4. Electron delocalization can affect the wavenumber of a functional group
5. Electron withdrawing/donating can affect the wavenumber of a functional group





lighter atom
bonded
carbon

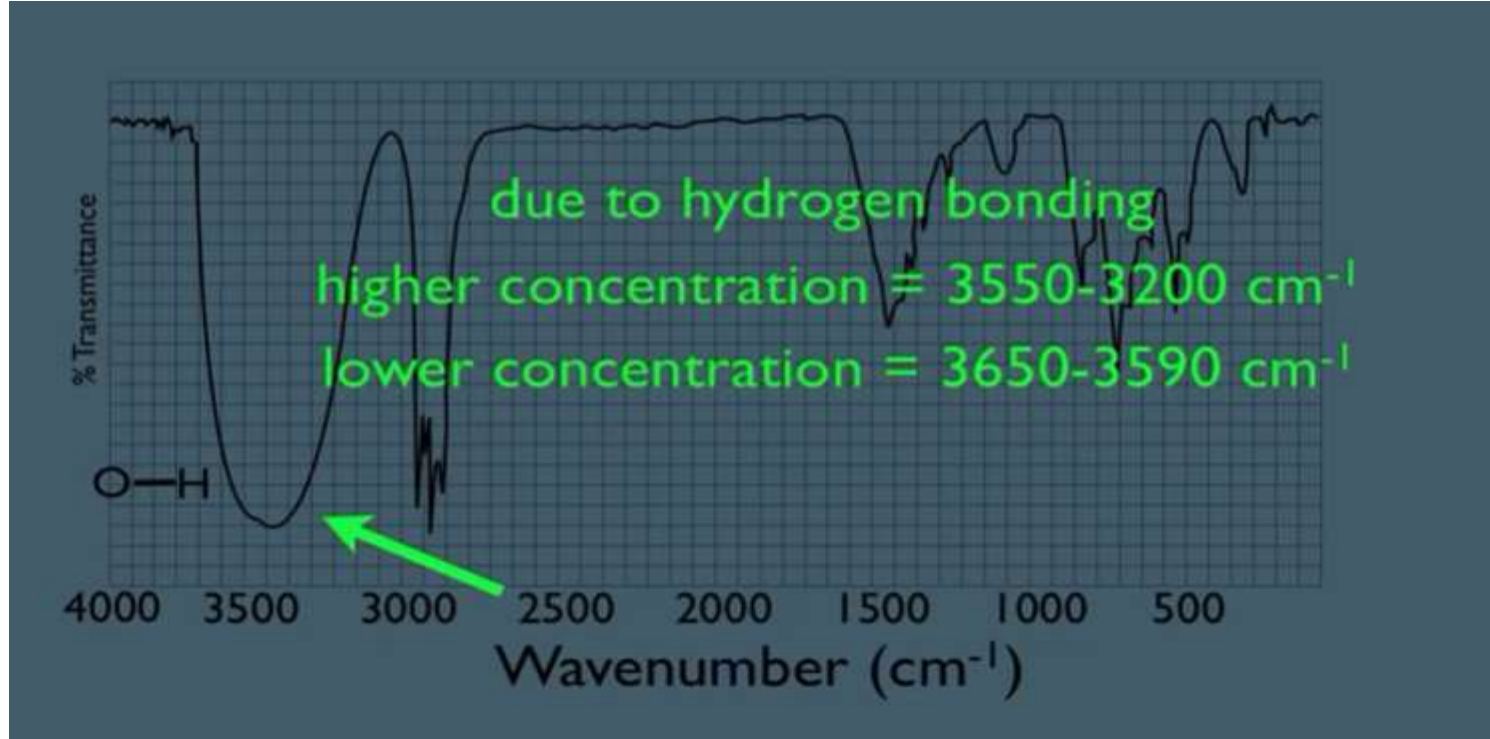


higher
wavenumber

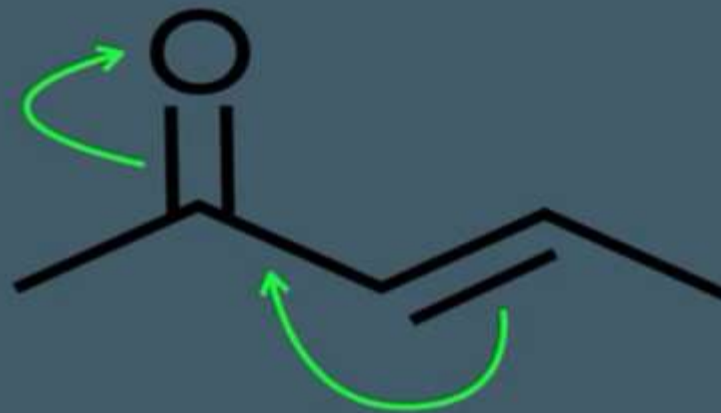
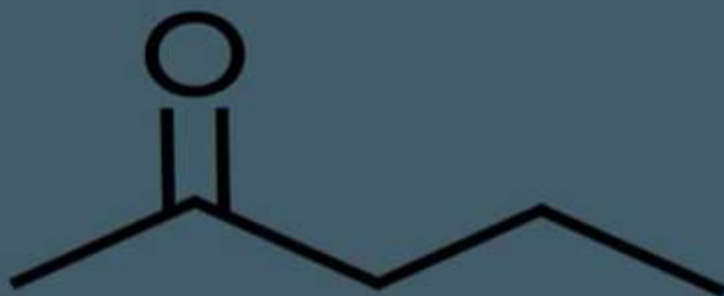


heaver atom
bonded
to carbon

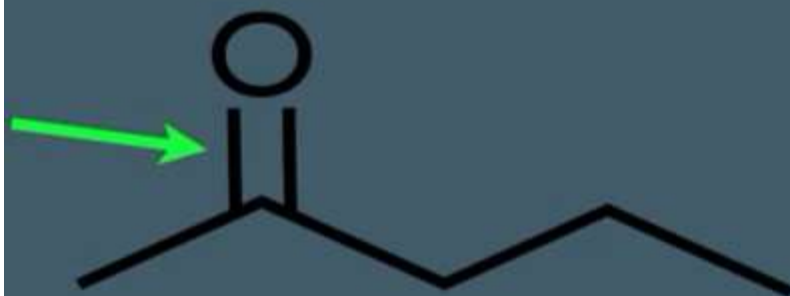
lower
wavenumber



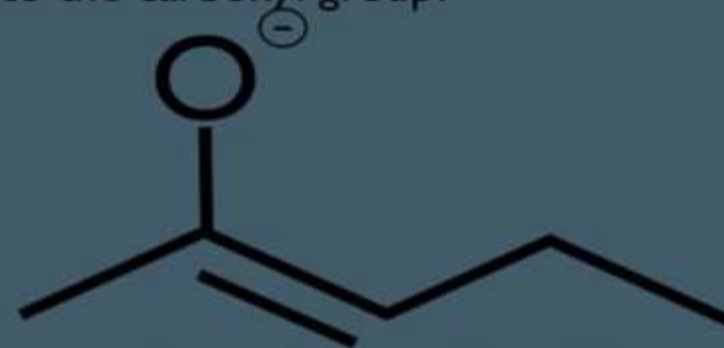
Sample Problem 1) In which molecule below would we observe a higher wavenumber due to the carbonyl group?



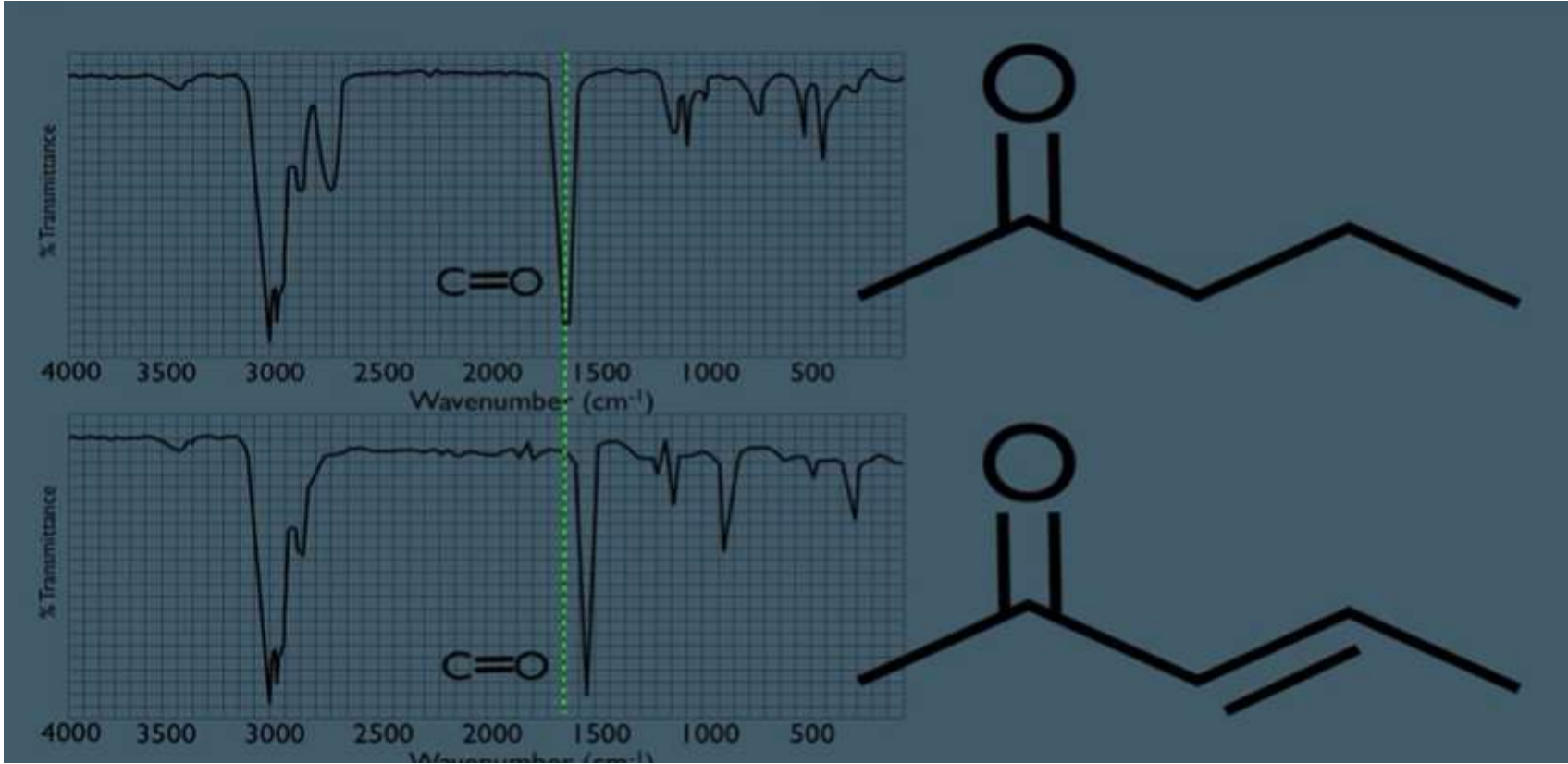
Sample Problem 1) In which molecule below would we observe a higher wavenumber due to the carbonyl group?



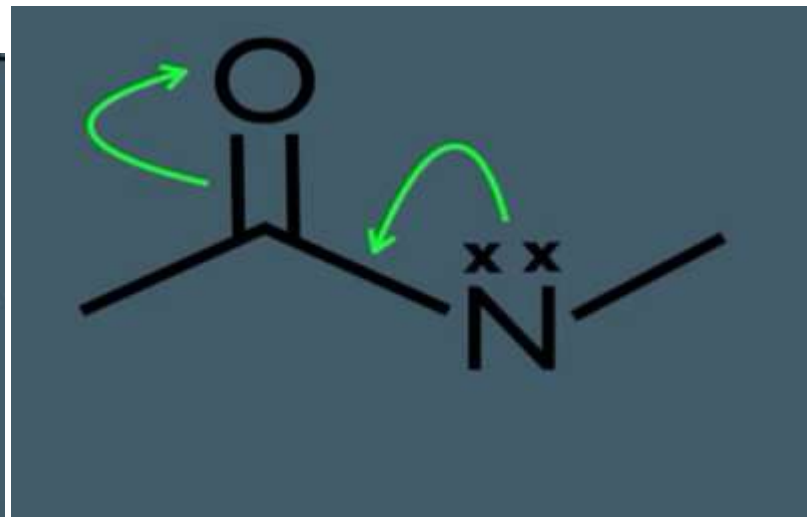
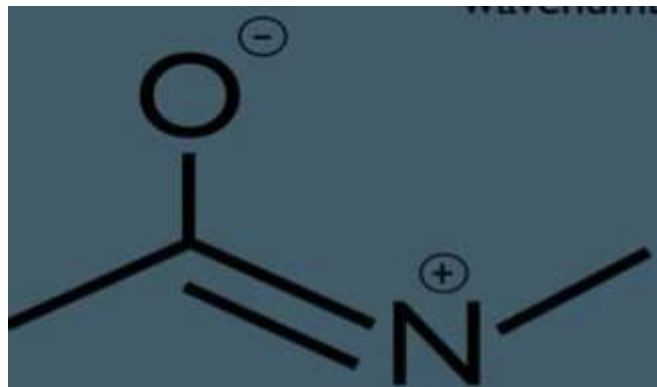
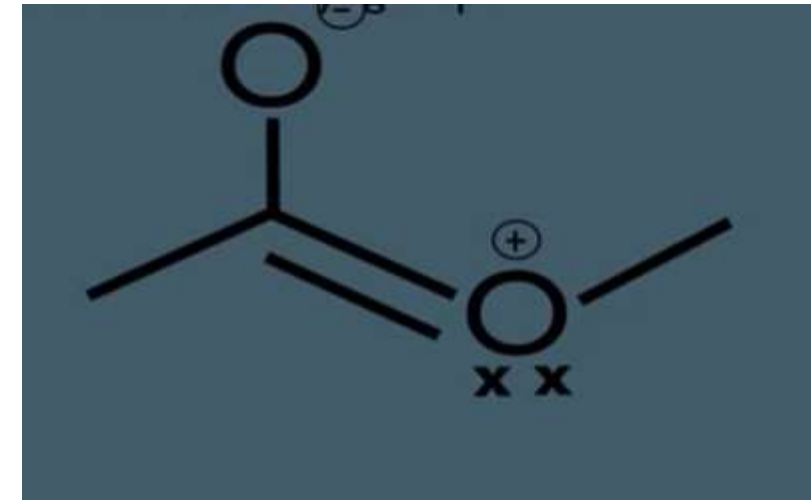
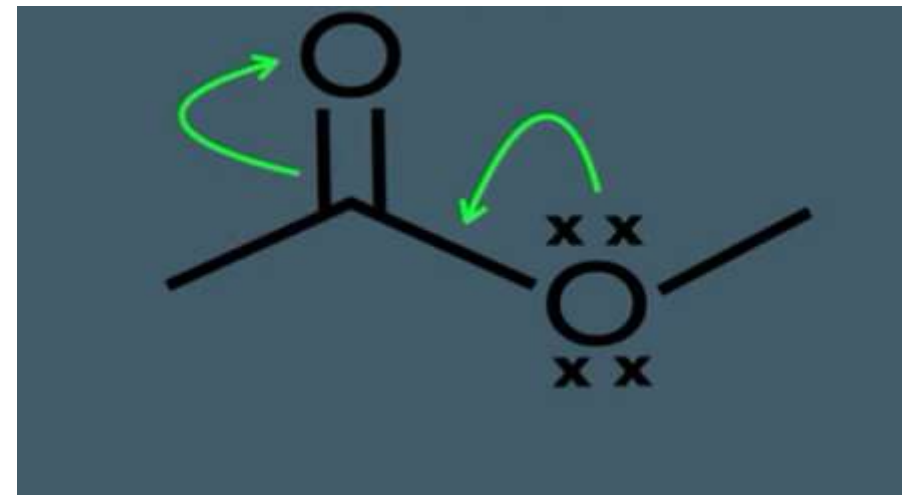
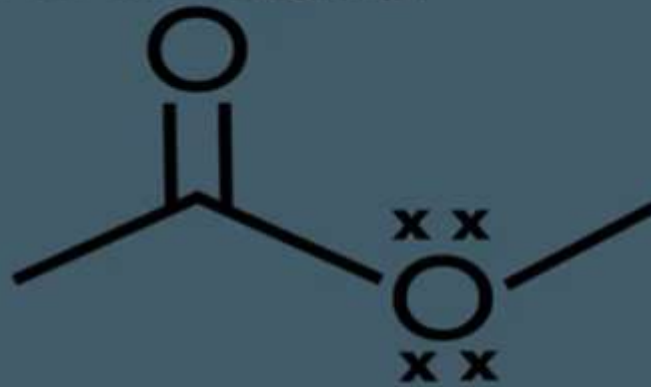
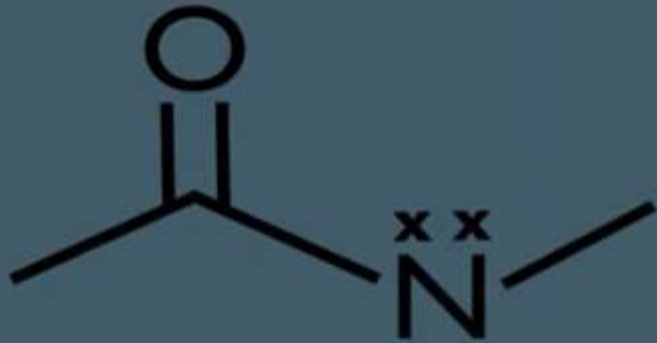
more double bond character
shorter bond
stronger bond
higher wavenumber



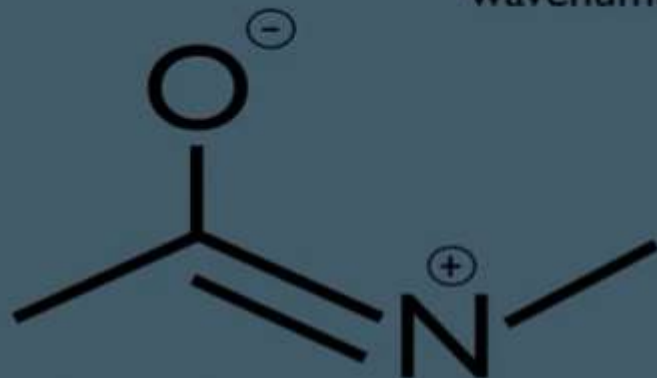
less double bond character
longer bond
weaker bond
lower wavenumber



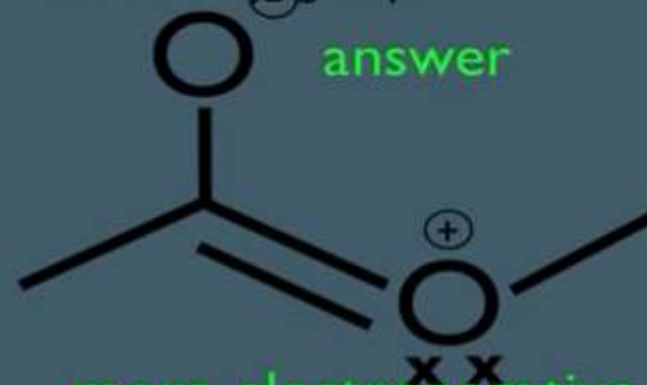
Sample Problem 2) In which molecule below would we observe a higher wavenumber due to the carbonyl group?



Sample Problem 2) In which molecule below would we observe a higher wavenumber due to the carbonyl group?



less electronegative
more electron donating
greater resonance
more single bond
character
lower wavenumber



more electronegative
less electron donating
less resonance
less single bond
character
higher wavenumber

