3. Problem on total theoretical mode of vibration:

Formula:

Total Theoretical mode of vibration = 3 N -5
for linear molecule

Total Theoretical mode of vibration = 3 N -6
for non-linear molecule

Where, N= total number of atom in molecule

for e.g.

Calculate total possible theoretical mode of vibration for ammonia (NH_3) molecule.

Soln:

Ammonia is sp^3 hybridized molecule hence it is non-linear

Therefore,

Total possible mode of vibration = 3 N – 6
= 3 x 4 -6
= 6

Calculate total possible modes of vibration in acetylene (c_2H_2)

Soln:

Acetylene is SP hybridized hence it is linear molecule

Therefore,

Total possible mode of vibration = 3 N -5 = 3 x 4 -5 = 7

Characteristic IR Absorption Frequencies of Organic Functional Groups

Functional Group	Type of Vibration	Characteristic Absorptions (cm-1)	Intensity
Alcohol			
O-H	(stretch, H-bonded)	3200-3600	strong, broad (free O-H will give sharp peak)
Alkane			
C-H	stretch	2850-3000	strong
-C-H	bending	1350-1480	variable
Alkene			
C=C	stretch	1620-1680	variable
Alkyne			
–C≡C–	stretch	2100-2260	variable, not present in symmetrical alkynes
Amine			
N-H	stretch	3300-3500	medium (primary amines have two bands; secondary have one band, often very weak)

Aromatic			
C=C	stretch	1400-1600	medium-weak, multiple bands

IR Absorption Frequencies of Functional Groups Containing a Carbonyl (C=O)

Functional Group	**Type of Vibration**	**Characteristic Absorptions (cm-1)**	**Intensity**
Carbonyl			
C=O	stretch	1670-1820	strong
(conjugation moves absorptions to lower wave numbers)			
Acid	(Peak for carbonyl +)		
O-H	stretch	2500-3300	strong, very broad
Aldehyde	(Peak for carbonyl +)		
=C-H	stretch	2820-2850 & 2720-2750	medium, two peaks
Ester	(Peak for carbonyl +)		
C-O	stretch	1000-1300	two bands or more

Functional Group	**Type of Vibration**	**Characteristic Absorptions (cm-1)**	**Intensity**
Ether			
C-O	stretch	1000-1300	strong
Nitrile			
- CN	stretch	2210-2260	medium