

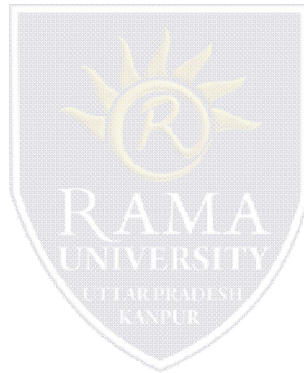


FACULTY OF ENGINEERING &
TECHNOLOGY

Infrared Spectroscopy

Content Outline

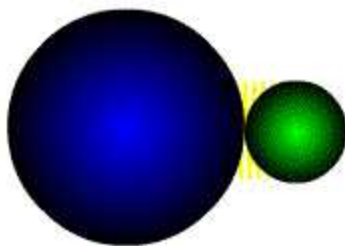
1. Infrared spectrscopy
2. Working & Instrumentation
3. Applications
4. Test your understanding
5. References & Further reading



Introduction

The IR Spectroscopic Process

1. The quantum mechanical energy levels observed in IR spectroscopy are those of *molecular vibration*
2. We perceive this vibration as heat
3. When we say a *covalent bond* between two atoms is of a certain length, we are citing an average because the bond behaves as if it were a vibrating spring connecting the two atoms
4. For a simple diatomic molecule, this model is easy to visualize:



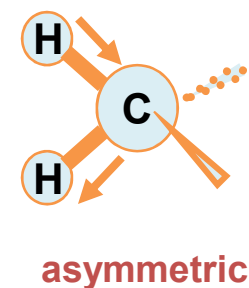
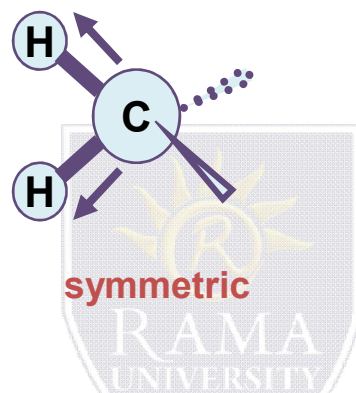
Vibration of a Diatomic Molecule
Approximates an Oscillating Spring

IR Spectroscopic process

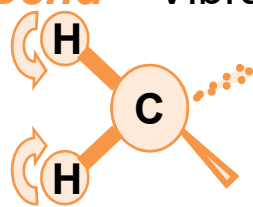
IR Spectroscopic Process

5. There are two types of bond vibration:

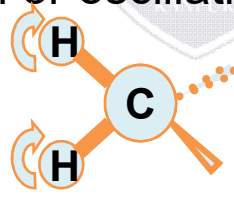
- **Stretch** – Vibration or oscillation along the line of the bond



- **Bend** – Vibration or oscillation not along the line of the bond

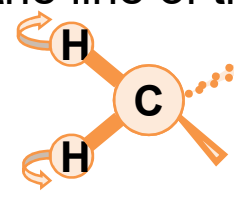


scissor

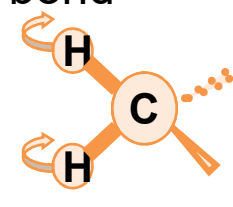


rock

in plane



twist

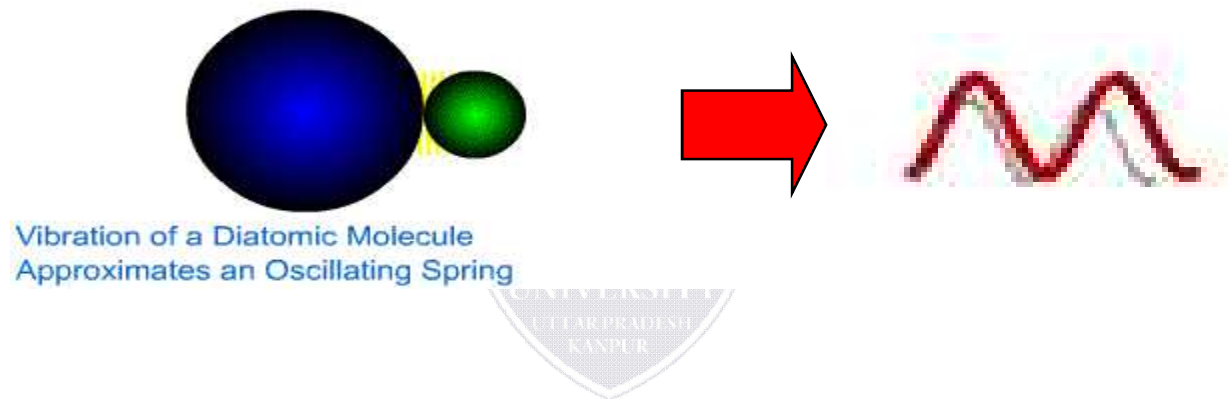


wag

out of plane



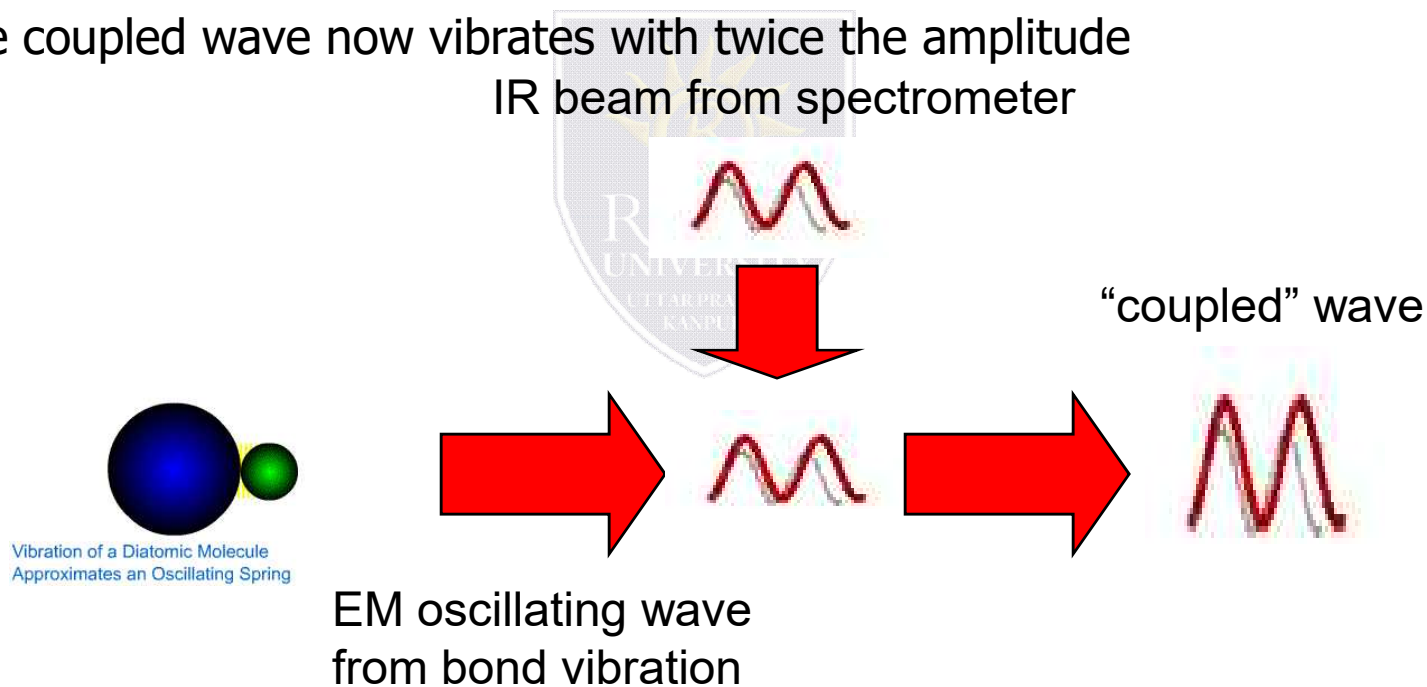
6. As a covalent bond oscillates – due to the oscillation of the dipole of the molecule – a varying electromagnetic field is produced



7. The greater the dipole moment change through the vibration, the more intense the EM field that is generated

8. When a wave of infrared light encounters this oscillating EM field generated by the oscillating dipole of the same frequency, the two waves couple, and IR light is absorbed

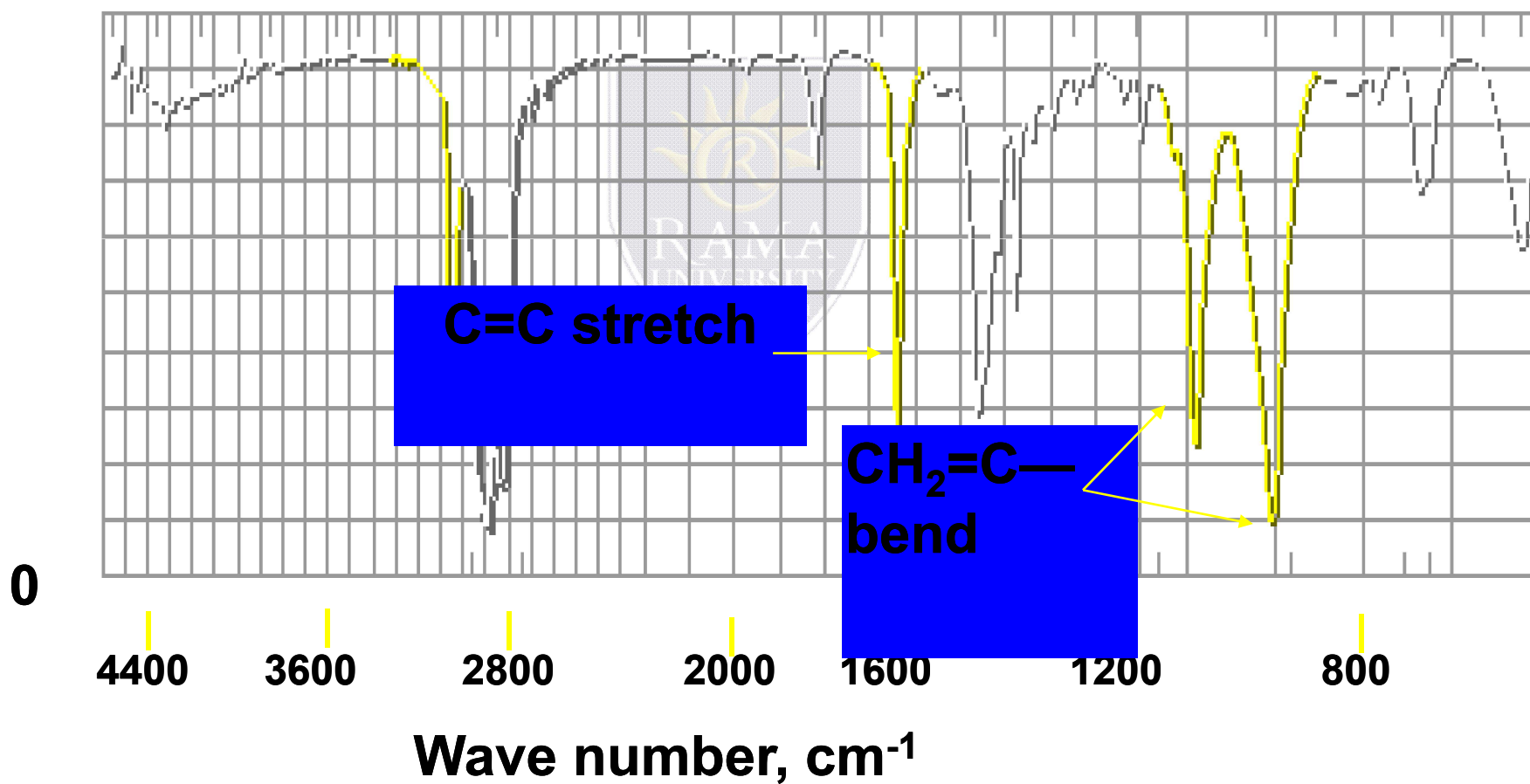
9. The coupled wave now vibrates with twice the amplitude
IR beam from spectrometer



Infrared spectrum of 1-hexene

Transmittance (%)

100



•Identification of functional group and structure elucidation

•Identification of substances

IR spectroscopy is used to establish whether a given sample of an organic substance is identical with another or not. This is because large number of absorption bands is observed in the IR spectra of organic molecules and the probability that any two compounds will produce identical spectra is almost zero. So if two compounds have identical IR spectra then both of them must be samples of the same substances.

IR spectra of two enantiomeric compound are identical. So IR spectroscopy fails to distinguish between enantiomers.

For example, an IR spectrum of benzaldehyde is observed as follows.

C-H stretching of aromatic ring-	3080 cm^{-1}
C-H stretching of aldehyde-	2860 cm^{-1} and 2775 cm^{-1}
C=O stretching of an aromatic aldehyde-	1700 cm^{-1}
C=C stretching of an aromatic ring-	1595 cm^{-1}
C-H bending-	745 cm^{-1} and 685 cm^{-1}

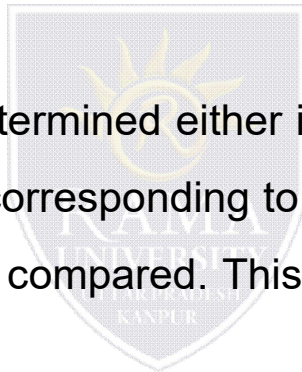
No other compound then benzaldehyde produces same IR spectra as shown above.

Detection of impurities

IR spectrum of the test sample to be determined is compared with the standard compound. If any additional peaks are observed in the IR spectrum, then it is due to impurities present in the compound.

Quantitative analysis

The quantity of the substance can be determined either in pure form or as a mixture of two or more compounds. In this, characteristic peak corresponding to the drug substance is chosen and $\log I_0/I_t$ of peaks for standard and test sample is compared. This is called base line technique to determine the quantity of the substance.



References & Further reading

1. Wilson, K, Walker, J., Principles and Techniques of Practical Biochemistry. 5th Ed. - Cambridge University Press,. Cambridge 1999.
2. Biotechniques, Theory & Practice: Second Edition by SVS Rana, Rustogi Publications.
3. Biochemical Methods of Analysis, Saroj Dua And Neera Garg : Narosa Publishing House, New Delhi.
4. Bioanalytical Techniques, M.L. Srivastava, Narosa Publishing House, New Delhi.

