Chapter-18
Infrared spectroscopy (FINGERPRINT REGION)

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Each trough (peak) is caused because energy is being absorbed from that particular frequency of infra-red radiation to excite bonds in the molecule to a higher state of vibration - either stretching or bending. Some of the troughs (peaks) are easily used to identify particular bonds in a molecule.

The following types of bond need to be recognised:-

Bond	Functional group	Absorbance (cm^{-1})
O - H	Alcohols	3200 - 3600 / strong and **broad***
O - H	Carboxylic acids	2500 - 3200 / medium and **very broad***
C=O	Aldehydes / ketones / carboxylic acids/ esters	1680 - 1750 / strong and sharp
C-O	Alcohols / esters / ethers	1050 - 1300 / medium
C-H	Alkanes / alkenes etc	2850 - 3100 / medium

*Broad due to Hydrogen Bonding between O-H groups

This is a typical infra-red spectrum:

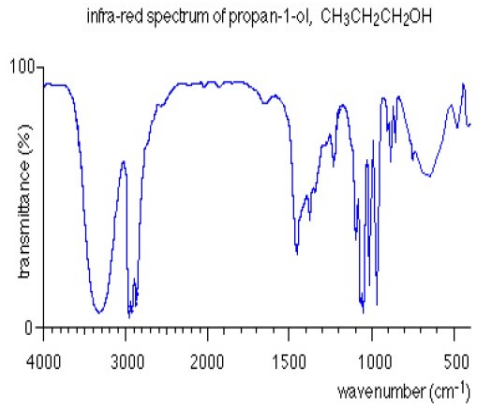

Fig.1. IR Spectrum of propan-1-ol ($CH_3CH_2CH_2OH$)

Here **(Fig.1),** the big trough (broad peak) at the left-hand side of the spectrum **3200-3600 cm^{-1}** is used to identify the presence of an oxygen-hydrogen **bond in an -OH group.**

The region to the right-hand side of the diagram (Fig.1) (from about 1500 to 400 cm^{-1}) usually contains a very complicated series of absorptions. These are mainly due to all manner of bending vibrations within the molecule. **This is called the fingerprint region.** It is much more difficult to pick out individual bonds in this region.

The importance of the fingerprint region is that each different compound produces a different pattern of peaks in this part of the spectrum.

USING THE FINGERPRINT REGION TO IDETIFY COMPOUNDS

The region between 400 cm^{-1} and 1500 cm^{-1} in the IR spectrum is known as the fingerprint region. Fingerprint region usually contains a large number of peaks, making it complicated to identify individual peaks. However, the fingerprint region of a given compound is distinctive and, therefore, can be used to differentiate between compounds.

Eg. Compare the infra-red spectra of propan-1-ol and propan-2-ol (Fig.2).

Both compounds contain exactly the same bonds. Both compounds have very similar peaks in the area around 3000 cm^{-1} but compare them in the fingerprint region between 1500 and 400 cm^{-1} as follows:

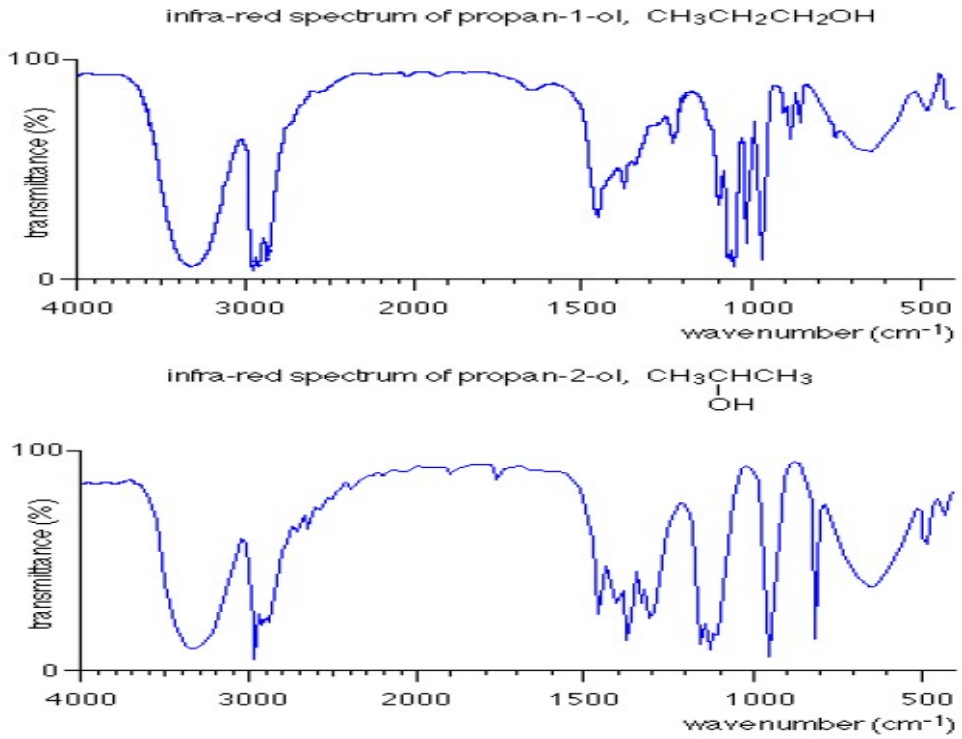

Fig.2. Comparative study of Finger Print Region in the infra-red spectra of propan-1-ol and propan-2-ol.

Both compounds contain exactly the same bonds. Both compounds have very similar troughs in the area around 3000cm^{-1} but compare them in the fingerprint region between 1500 and 400cm^{-1}. **The pattern in the fingerprint region is completely different and could therefore be used to identify the positional isomers, propan-1-ol and propan-2-ol.**

To positively identify an unknown compound, use its infra-red spectrum to identify what sort of compound it is by looking for specific bond absorptions. That might tell you, for example, that you had an alcohol because it contained an -OH group. You would then compare the fingerprint region of its infra-red spectrum with known spectra measured under exactly the same conditions to find out which alcohol (or whatever) you had.

Related Questions:

Q.1. What is finger print region? Discuss its utility in the IR spectrum.

Q.2. How do you differentiate positional isomers through finger print region?

Reference Books:

1. Fourier Transforms in NMR, Optical and Mass Spectroscopy, Alan G. Marshall, Francis R. Verdun, Elsevier, 1990.

2. Practical Fourier Transform Infrared Spectroscopy, John R. Ferraro, K. Krishnan, Academic Press, 1990

3. Infrared Spectroscopy: Fundamentals and Applications, Barbara H. Stuart, John Wiley & Sons, Ltd, 2004.

4. Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A: Theory and Applications in Inorganic Chemistry, Sixth Edition, Kazuo Nakamoto, John Wiley & Sons, Ltd, 2008.

5. Infrared and Raman spectroscopy principles and spectral interpretation, Peter Larkin, Elsevier, 2011.
