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Study of the composition of carboxylic compounds using ir spectroscopy

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Abstract
In this article, we determined the chemical composition of the following compounds using IR spectroscopy: 2-butanone, butyl aldehyde, benzaldehyde, ethyl acetate, ethyl benzoate, benzoic acid. The absorption spectrum of 2-butanone is between the wave numbers 2991 cm^{-1} and 1715 cm^{-1}. The absorption spectrum of butyl aldehyde is between the wave numbers 2976 cm^{-1} and 1731 cm^{-1}. The absorption spectrum of benzaldehyde is between the wave numbers 3073 cm^{-1} and 1696 cm^{-1}. The absorption spectrum of ethyl acetate is between the wave numbers 2981 cm^{-1} and 1055 cm^{-1}. The absorption spectrum of ethyl benzoate is between the wave numbers 3078 cm^{-1} and 1117 cm^{-1}. The absorption spectrum of benzoic acid is between the wave numbers 2971 cm^{-1} and 948 cm^{-1}.

Keywords: 2-butanone, butyl aldehyde, benzaldehyde, ethyl acetate, ethyl benzoate, benzoic acid

Introduction

The absorption of electromagnetic radiation at wavelengths between 0.8 and 1000 μm is attributed to the infrared (IR) range of the spectrum. More significant information from an analytical point of view is provided by the mid-IR range, also called fundamental IR (λ=2.5 – 25 μm) [1-5].

The first commercial instruments for the IR range appeared as early as the 1940s. The diversity of devices used today in the most diverse fields can be divided into three categories: non-dispersive photometers based on simple filters sometimes formed even from the gases to be analyzed; spectrometers based on light dispersion (using prisms or monochromators based on diffraction and interference); spectrometers based on the Fourier transform, which allow the entire spectral range to enter the cell and which detect the characteristic absorption lines interferometrically. These instruments, due to their better resolution and speed, due to the coupling with the computer, have recently become preferred (fig. 1) [6-8].

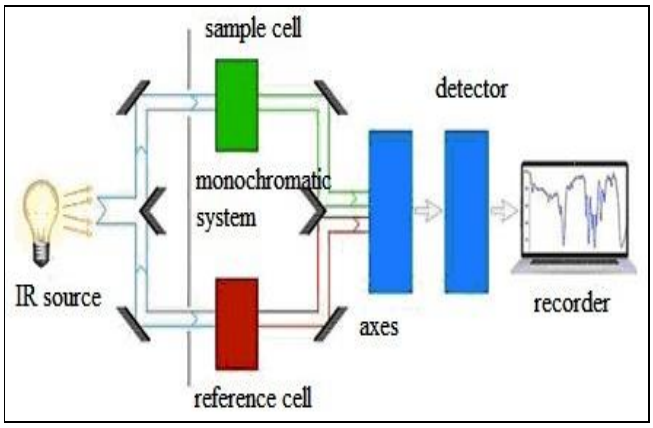

Fig 1: Schematic diagram of an IR spectrophotometer

IR radiation sources can include W filament bulbs (for near IR), Nernst tubes, Globar lamps and Nichrome filaments for fundamental IR and high-pressure mercury lamps for far IR. IR monochromators are built on the same principles as those in the UV-VIS range and can be prism or grating.

Detectors used in IR absorption spectrometry are distinct from the rest of the detectors used in UV-VIS. They can be classified based on the principle underlying their operation into two groups: quantum detectors, based on the effect of photons on materials; and thermal detectors, which are based on the change in the physical properties of materials with temperature [9-18].

Material and methods

Figure 2 shows the equipment necessary to determine the FTIR spectrum of carboxylic compounds.

Fig 2: Nicolet Avatar FTIR Spectrometer

Results and Discussion

The carbonyl stretching vibration band C=O of saturated aliphatic ketones appears at 1715 cm^{-1}. Conjugation of the carbonyl group with carbon-carbon double bonds or phenyl groups, as in alpha, beta-unsaturated aldehydes and benzaldehyde, shifts this band to lower wavenumbers, 1685-1666 cm^{-1}.

Summary

- C=O stretch
- aliphatic ketones 1715 cm^{-1}
- α, β-unsaturated ketones 1685-1666 cm^{-1}

The spectrum of 2-butanone is shown below. This is a saturated ketone, and the C=O band appears at 1715 cm^{-1}. Note the C–H stretches (around 2991 cm^{-1}) of alkyl groups ($–CH_3$). It's usually not necessary to mark any of the bands in the fingerprint region (less than 1500 cm^{-1}).

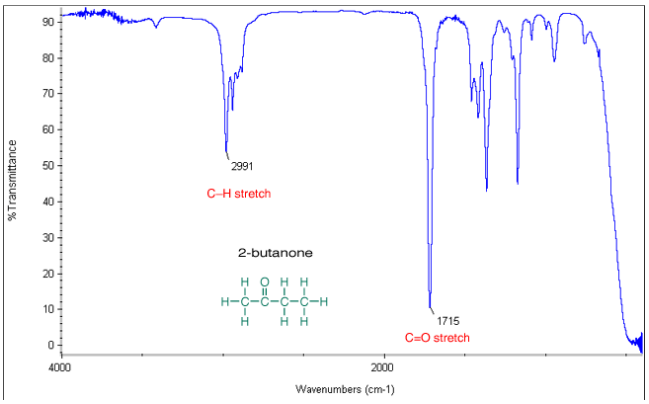

Fig 3: IR spectrum for 2-butanone

The carbonyl stretch C=O of saturated aliphatic aldehydes appears from 1730-1720 cm^{-1}. As in ketones, if the carbons adjacent to the aldehyde group are unsaturated, this vibration is shifted to lower wavenumbers, 1710-1685 cm^{-1}. Another useful diagnostic band for aldehydes is the O=C–H stretch. This band generally appears as one or two bands of moderate intensity in the region 2830-2695 cm^{-1} (typically at 2720 cm^{-1}). Since the band near 2830 cm-1 is usually indistinguishable from other C–H stretching vibration bands (recall that the C–H stretches of alkanes appear from 3000-2850 cm^{-1}), the presence of a moderate band near 2720 cm^{-1} is more likely to be helpful in determining whether or not a compound is an aldehyde. If you suspect a compound to be an aldehyde, always look for a peak around 2720 cm^{-1}; it often appears as a shoulder-type peak just to the right of the alkyl C–H stretches.

Summary

- H–C=O stretch 2830-2695 cm^{-1}; (typically at 2720 cm^{-1})
- C=O stretch
- aliphatic aldehydes 1735-1720 cm^{-1}
- alpha, beta-unsaturated aldehydes 1710-1685 cm^{-1}

Table 1: Peak assignment in the FTIR spectrum of 2-butanone

Wave number, cm^{-1}	Functional grouping	Vibration mode
2991	C-H	stretch
1715	C=O	stretch

The spectrum of butyraldehyde is shown below. Note the O=C–H stretches in the region 2830-2695 cm^{-1}, especially the shoulder peak at 2725 cm^{-1} in butyraldehyde.

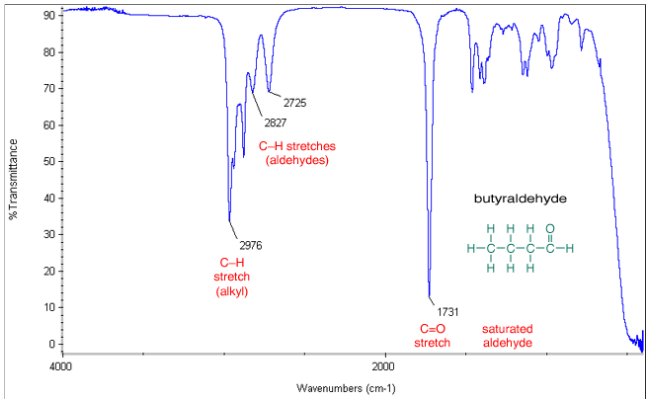

Fig 4: IR spectrum for butyl aldehyde

Table 2: Peak assignment in the FTIR spectrum of butyl aldehyde

Wave number, cm^{-1}	Functional grouping	Vibration mode
2976	C-H	Stretch (alkyl)
2827	C-H	Stretches (aldehydes)
2725	C-H	Stretches (aldehydes)
1731	C=O	Stretch (saturated aldehydes)

The carbonyl stretch C=O of aliphatic esters appears from 1750-1735 cm^{-1}; that of α, β-unsaturated esters appears from 1730-1715 cm^{-1}.

The C–O stretches appear as two or more bands in the region 1300-1000 cm-1.

Summary

- C=O stretch
- aliphatic from 1750-1735 cm^{-1}
- α, β-unsaturated from 1730-1715 cm^{-1}
- C–O stretch from 1300-1000 cm^{-1}

The spectrum of ethyl acetate is shown below. Note that the C=O stretch of ethyl acetate (1752 cm^{-1}) is at a higher wavelength than that of the α, β-unsaturated ester ethyl benzoate (1726 cm^{-1}).

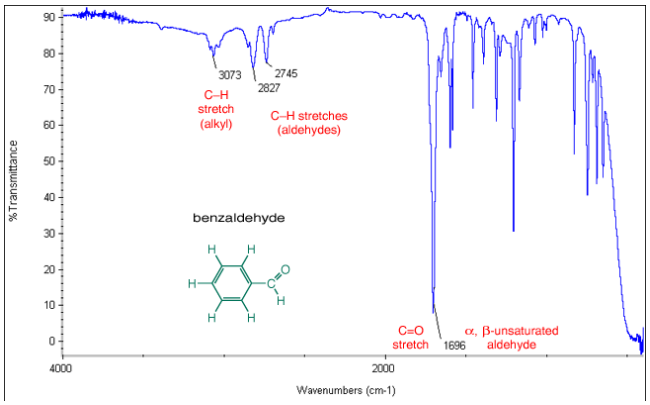

Fig 5: The IR spectrum of benzaldehyde

Table 3: Peak assignment in the FTIR spectrum of benzaldehyde

Wave number, cm^{-1}	Functional grouping	Vibration mode
3073	C-H	stretch (alkyl)
2827	C-H	stretches (aldehydes)
2745	C-H	stretches (aldehydes)
1696	C=O	stretch(α, β-unsaturated aldehyde)

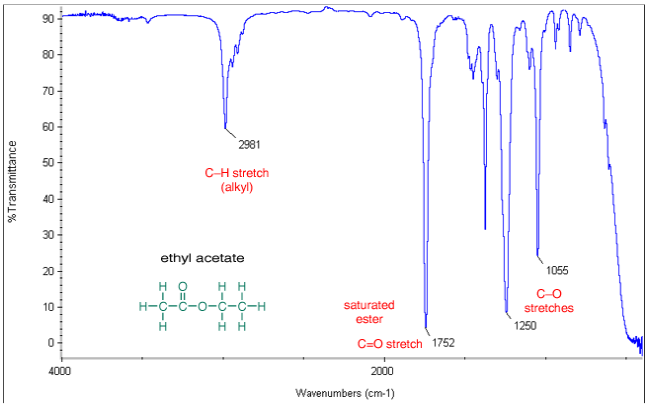

Fig 6: IR spectrum for ethyl acetate

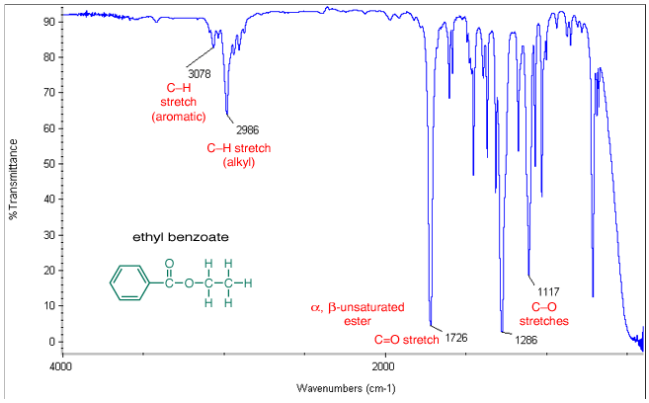

Fig 7: IR spectrum for ethyl benzoate

Carboxylic acids show a strong, wide band for the O–H stretch. Unlike the O–H stretch band observed in alcohols, the carboxylic acid O–H stretch appears as a very broad band in the region 3300-2500 cm^{-1}, centered at about 3000 cm^{-1}. This is in the same region as the C–H stretching bands of both alkyl and aromatic groups. Thus a carboxylic acid shows a somewhat "messy" absorption pattern in the region 3300-2500 cm^{-1}, with the broad O–H band superimposed on the sharp C–H stretching bands. The reason that the O–H stretch band of carboxylic acids is so broad is becase carboxylic acids usually exist as hydrogen-bonded dimers.

The carbonyl stretch C=O of a carboxylic acid appears as an intense band from 1760-1690 cm-1. The exact position of this broad band depends on whether the carboxylic acid is saturated or unsaturated, dimerized, or has internal hydrogen bonding. The C=O stretch band of dimerized aliphitic acid is typically localized between 1720-1710 cm^{-1}.

The C–O stretch appears in the region 1320-1210 cm-1, and the O–H bend is in the region 1440-1395 cm^{-1} and 950-910 cm^{-1}, although the 1440-1395 band may not be distinguishable from C–H bending bands in the same region.

Summary

- O–H stretch from 3300-2500 cm^{-1}
- C=O stretch from 1760-1690 cm^{-1} (aliphatic: typically localized between 1720-1710 cm^{-1})
- C–O stretch from 1320-1210 cm^{-1}
- O–H bend from 1440-1395 and 950-910 cm^{-1}

Table 4: Peak assignment in the FTIR spectrum of ethyl acetate

Wave number, cm^{-1}	Functional grouping	Vibration mode
2981	C-H	stretch (alkyl)
1752	C=O	Stretch (saturated ester)
1250	C-O	Stretches
1055	C-O	Stretches

The spectrum of hexanoic acid is shown below. Note the broad peak due to O–H stretch superimposed on the sharp band due to C–H stretch. Note the C=O stretch (1721 cm^{-1}), C–O stretch (1296 cm^{-1}), O–H bends (1419, 948 cm^{-1}).

Table 5: Peak assignment in the FTIR spectrum of ethyl benzoate

Wave number, cm^{-1}	Functional grouping	Vibration mode
3078	C-H	stretch (aromatic)
2966	C-H	stretch (alkyl)
1726	C=O	stretch(α, β-unsaturated ester)
1286	C-O	Stretches
1117	C-O	Stretches

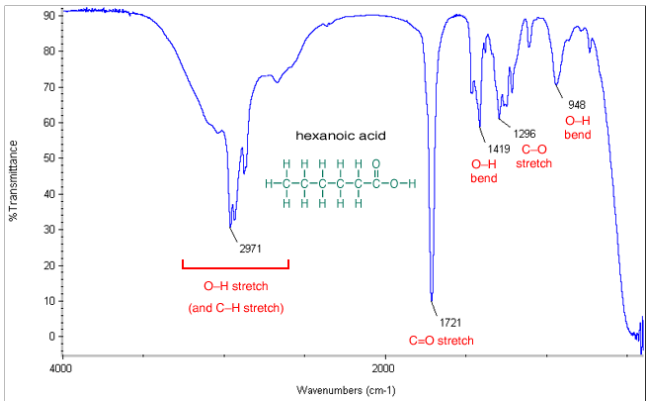

Fig 8: IR spectrum of hexanoic acid

Table 6: Peak assignment in the FTIR spectrum of hexanoic acid

Wave number, cm^{-1}	Functional grouping	Vibration mode
2971	C-H	stretch
1971	O-H	stretch
1721	C=O	stretch
1419	O-H	bend
1296	C-O	stretch
948	O-H	bend

Conclusions

2-butanone contains in IR only bands characteristic of functional groups: alkanes and carbonyls. Butyl aldehyde contains in IR only bands characteristic of functional groups: alkanes and carbonyls. Benzaldehyde contains in IR only bands characteristic of functional groups: aldehydes, saturated aliphatic. Ethyl acetate contains in IR only bands characteristic of functional groups: alpha,beta–unsaturated esters. Ethyl benzoate contains in IR only bands characteristic of functional groups: alpha,beta–unsaturated esters. Benzoic acid contains in IR only bands characteristic of functional groups: carboxylic acids.

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