

Chemistry 264

Practical 6

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Abstract

In this practical the use of IR spectroscopy to identify molecules and their substituent functional groups was investigated.

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1 Introduction

In this practical we aim to identify six different compounds by way of IR spectroscopy.

IR spectroscopy enables the measurement of the absorbance/transmittance of a sample over a region of the IR spectrum. The region measured in this practical is the mid-IR($4000 - 400 \text{ cm}^{-1}$), which reveals the resonant frequencies of the molecules being analysed, from this the molecules may be characterised. Specifically peaks at particular frequencies indicate the presence of different bond types, from which the substituent functional groups of a molecule may be identified. Allowing for the molecule to be easily identified, if a reference spectrograph is available, or at least for the molecule to be characterised and differentiated from other samples.

2 Experiment

A variety of sample preparation techniques are available, among those are the following.

Mulling

The sample is ground into a fine powder with a mortar and pestle, and mixed with a mulling agent, in this case the mineral oil Nujol. It is then further ground into a paste, and then placed between two plates, that may be squeezed together to achieve the desired thickness of mull. [1]

Pellet method

The sample is ground with Potassium bromide. This mixture is then compressed with a press into a compacted pellet. The sample can then be analysed unhindered by the presence of the Potassium bromide as it is transparent in the IR region being sampled.[1]

Liquid Samples

Liquid samples may be directly placed in a cell composed of two plates, transparent to IR.

3 Results

Find below table 1 through table 6 showing the bonds identified in each sample and their associated wavenumber, from which the molecules were identified.[2][3][4]

Table 1: A - Benzaldehyde

Bond	Wavenumber (cm^{-1})
C-H benzene	3050
C-H aldehyde	2800 & 2750
C=O aldehyde α, β unsaturated	1700
C-H monosub benzene	750 & 700
C-H trisub. alkene	850

Table 2: B - 3-Nitroaniline

Bond	Wavenumber (cm^{-1})
C=C	1650
N-O aromatic nitro	1550 & 1350

Table 3: C - Diethyl phthalate

Bond	Wavenumber (cm^{-1})
C-H benzene	3000
C-H methyl	2950 & 2850
C=O ester	1750
C=C aromatic	1610 & 1590 & 1500 & 1450
C-O ester	1300
C-H meta-disub. benzene	850 & 750

Table 4: D - 4-Aminobenzoic acid

Bond	Wavenumber (cm^{-1})
N-H primary amine	3450 & 3350
C=O carboxylic acid	1680
C=N	1650
C=C aromatic	1600 & 1550 & 1500 & 1450
C-O carboxylic acid	1300
C-H para-disub. benzene	850

Table 5: E - Benzamide

Bond	Wavenumber (cm^{-1})
N-H primary amine	3350
C-H benzene	3050
C=O aromatic ketone	1650

Table 6: F - THF

Bond	Wavenumber (cm^{-1})
C-H	2950 & 2850 & 1400
C-O aliphatic ether	1100

4 Conclusion

IR spectroscopy has been shown to be an extremely accurate and consistent method of identification and characterisation of a wide range of organic molecules.

References

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- ³P. Larkin, *Infrared and raman spectroscopy: principles and spectral interpretation* (Elsevier, Amsterdam ; Boston, 2011), 228 pp.
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