

Spectroscopy Revision Helpsheet

Lesson Objective	Task(s)		
Understand that the fragmentation of a molecular ion gives rise to a characteristic relative abundance spectrum that may give information about the structure of the molecule	What is a molecular ion?	Explain what fragmentation is and write an equation to represent it.	Explain how fragmentation patterns can be used to give information about the structure of a molecule.
Know that the more stable X ⁺ species give higher peaks, limited to carbocation and acylium (RCO ⁺) ions	Describe how the relative abundance of a peak is related to the stability of the cation	Compare the stability of primary, secondary and tertiary carbocations.	Explain why acylium ions are stable fragments.
Be able to use IR spectra to identify functional groups.	State the range of the 'fingerprint' region.	Explain what the fingerprint region is.	Describe the similarities and differences between the IR spectra of alcohols, carbonyls, esters and carboxylic acids.
Understand that nuclear magnetic resonance gives information about the position of ¹³ C or ¹ H atoms in a molecule	Describe what is meant by shielding.	Describe how shielding influences the chemical shift of an atom.	
Understand that ¹³ C n.m.r. gives a simpler spectrum than ¹ H n.m.r.	State the percentage of 'natural' carbon that is ¹³ C.	Explain why spin-spin coupling is seen in ¹ H nmr but not in ¹³ C nmr.	
Know the use of the δ scale for recording chemical shift	State the typical range of the δ scale for ¹ H nmr.	State the typical range of the δ scale for ¹³ C nmr.	State what chemical shift is and the unit it is measured in.
Understand that chemical shift depends on the molecular environment	Describe how the molecular environment influences the chemical shift of an atom.		

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Understand how integrated spectra indicate the relative numbers of ^1H atoms in different environments	What information can we get from the area under a peak?	Sketch a typical integration trace.	Describe how an integration trace can be used to calculate the ratio of the atoms causing a signal.
Understand that ^1H n.m.r. spectra are obtained using samples dissolved in proton-free solvents	What would happen if an nmr sample was dissolved in a solvent that contained protons?	Explain why deuterated solvents are commonly used in for nmr samples.	State four solvents that could be used for an nmr sample.
Understand why tetramethylsilane (TMS) is used as a standard	Explain why a standard is necessary in nmr spectra.	Draw the structure of tms.	State 5 reasons why tms is a suitable standard for nmr.
Be able to use the $n + 1$ rule to deduce the spin-spin splitting patterns of adjacent, non-equivalent protons, limited to doublet, triplet and quartet formation in simple aliphatic compounds	Explain why spin-spin coupling happens.	State the $n + 1$ rule.	How many adjacent protons are needed to create a doublet triplet and quartet.
Know that gas-liquid chromatography can be used to separate mixtures of volatile liquids	Sketch a typical trace obtained from gas-liquid chromatography.	Describe what information can be obtained from a gas-liquid chromatography trace.	State three common applications of gas-liquid chromatography.
Know that separation by column chromatography depends on the balance between solubility in the moving phase and retention in the stationary phase	Sketch and label the equipment used for gas chromatography.	Describe what the mobile and stationary phases are.	Explain how the retention time of a chemical is influenced by its solubility.
Be able to use data from mass spectroscopy, infra-red, nmr and chromatography to determine the structure of specified compounds	Describe how to use data from mass spectroscopy, infra-red, nmr and chromatography to determine the structure of specified compounds		

