AQA Chemistry A-level
Topic 3.15 - NMR Spectroscopy

Flashcards

What does NMR stand for?

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Nuclear Magnetic Resonance

What are the basic principles of NMR?

What are the basic principles of NMR?

You can find the structures of complex molecules by placing them in a magnetic field and applying EM waves of radio frequency to them. If radio waves of the right frequency are absorbed, the nuclei flips from parallel to applied magnetic to field to anti-parallel. This energy change can be monitored and recorded. Uses the resonance of nuclei with spin.

How would you carry out NMR spectroscopy?

How would you carry out NMR spectroscopy?

Dissolve the liquid sample in suitable solvent, put in a tube along with a small amount of TMS and put the tube into an NMR machine. The sample is spun to even out any imperfections in the magnetic field and the spectrometer is zeroed against the TMS. Radiation with different radio frequencies but a constant magnetic field is applied to the sample and any absorptions (due to resonance) are detected

Give one use of NMR?

Give one use of NMR?

MRI scans

What kind of nuclei does NMR work with (and examples)?

What kind of nuclei does NMR work with (and examples)?

Those with an uneven number of nucleons, meaning they will spin e.g. ^1H, ^{13}C

What percentage of carbon atoms are ^{13}C?

What percentage of carbon atoms are ^{13}C?

1% - but modern instruments are sensitive enough to detect this

What defines the resonant frequency of a ^{13}C atom?

What defines the resonant frequency of a ^{13}C atom?

The chemical environment that it is in; the amount of electron shielding it has.

What graph is produced by NMR spectroscopy?

What graph is produced by NMR spectroscopy?

Energy absorbed against chemical shift

What is chemical shift? What is its symbol? What are its units?

What is chemical shift? What is its symbol? What are its units?

The resonant frequency of the nuclei, compared to that of a ^{1}H atom in TMS.

Symbol δ

Parts per million (ppm)

What is the range of chemical shift for ^{13}C NMR?

What is the range of chemical shift for ^{13}C NMR?

0-200ppm

What means ^{13}C atoms show a different chemical shift value?

What means ^{13}C atoms show a different chemical shift value?

Having different chemical environments (but equivalent atoms show the same peak)

What kind of environment leads to a greater chemical shift?

What kind of environment leads to a greater chemical shift?

A C atom next to more electronegative atom has a greater chemical shift.

Summarise what these mean for ^{13}C NMR:

Number of signals?
Chemical shift?
Area under peak?
Splitting?

Summarise what these mean for ^{13}C NMR:

Number of signals: One signal for each carbon environment (each set of inequivalent ^{13}C atoms)

Chemical shift: Greater ⬚ from atoms closer to electronegative atoms or C=C

Area under peak: no meaning

Splitting: there is no splitting for ^{13}C NMR

Why is it easier to get a spectrum of ^{1}H NMR than ^{13}C NMR?

Why is it easier to get a spectrum of ^{1}H NMR than ^{13}C NMR?

Most H atoms are ^{1}H- it is much more abundant than ^{13}C. This means almost all H atoms have spin so show up

What is the range of chemical shift for ^{1}H NMR?

What is the range of chemical shift for ^{1}H NMR?

0-10ppm

What leads to a lower chemical shift value for H NMR?

What leads to a lower chemical shift value for H NMR?

^{1}H with more electrons around them i.e. further from electronegative groups/atoms

On a low resolution spectrum, what peaks would you expect to see for H NMR?

On a low resolution spectrum, what peaks would you expect to see for H NMR?

One peak for each set of inequivalent H atoms

(each chemical environment shows 1 peak)

What does the area under the peak represent (for H NMR)?

What does the area under the peak represent (for H NMR)?

The area under the peak is proportional to the number of ^{1}H atoms represented by the peak

What is the integration trace?

What is the integration trace?

A stepped line that makes it easier to measure the area under the curve (height of line = area under that peak)

What is TMS (name and structure)?

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Tetramethylsilane
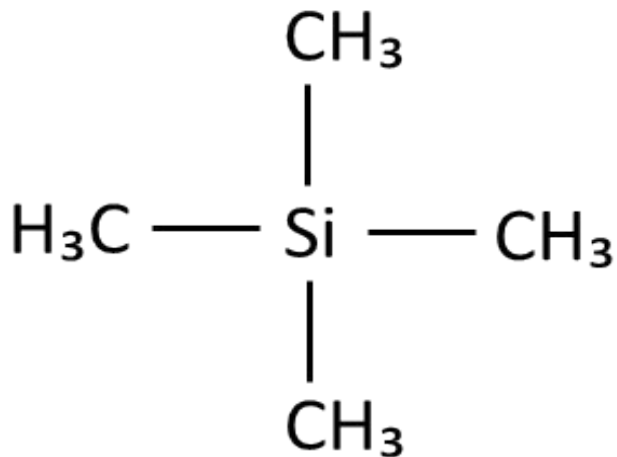
What state is TMS at room temperature?

What state is TMS at room temperature?

liquid

Why is TMS used?

Why is TMS used?

Can be added to sample to calibrate the NMR equipment. It provides a peak at exactly δ = 0ppm. It is the reference point against which all δ are measured

What are other advantages of using TMS?

What are other advantages of using TMS?

Inert, non-toxic, easy to remove from the sample (as relatively volatile)

When does splitting/spin-spin coupling occur?

When does splitting/spin-spin coupling occur?

Neighbouring hydrogen atoms (3 or fewer bonds away, or on the adjacent carbon) affect the magnetic field of ^{1}H atoms and causes their peaks to split

What is the n+1 rule?

What is the n+1 rule?

If there are n inequivalent ^{1}H atoms on the neighbouring carbon then the peak will split into (n+1) smaller peaks

Draw the splitting patterns for 0, 1, 2 and 3 inequivalent H atoms 3 bonds or less away

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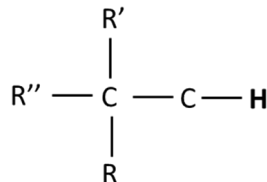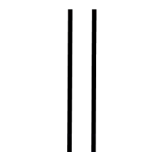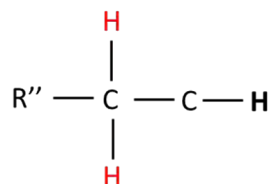

No coupled protons — Singlet
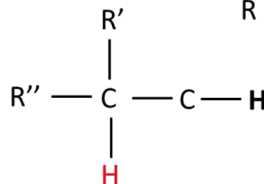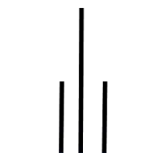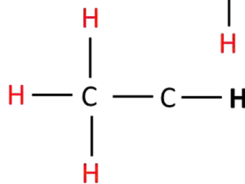
One coupled proton — Doublet

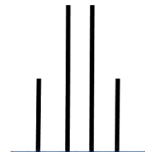**Two coupled protons** — Triplet

Three coupled protons — Quartet

Why must solvents used for ^{1}H NMR not contain any hydrogen atoms?

Why must solvents used for ^{1}H NMR not contain any hydrogen atoms?

Signals from the solvent would swamp signals from the sample, as there is much more solvent than sample.

Which solvents are used?

Which solvents are used?

Deuterated solvents: $CDCl_3$, D_2O, C_6D_6

CCl_4 - tetrachloromethane

Summarise what these indicate for ^{1}H NMR:

Number of signals?
Chemical shift?
Splitting?
Area under peak?

Summarise what these indicate for ¹H NMR:

Number of signals: One main signal for each set of inequivalent ¹H atoms (for each hydrogen environment)

Chemical shift: Larger ☐ for ¹H atoms closer to electronegative atoms or C=C

Splitting: Number of smaller peaks = 1 + number of inequivalent hydrogen atoms 3 bonds away

Area under peak: Proportional to the number of atoms represented by that peak

Why does the peak from O-H bonds disappear if D_2O is used as a solvent?

Why does the peak from O-H bonds disappear if D_2O is used as a solvent?

O-D bond is formed in preference to O-H due to labile protons that move/swap from one molecule to another.