OCR (A) Chemistry A-level

Topic 6.3.2 - Spectrometry

Flashcards

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What does NMR stand for?

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What does NMR stand for?

Nuclear Magnetic Resonance

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What are the basic principles of NMR?

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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.

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Give one use of NMR?

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Give one use of NMR?

MRI scans

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

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

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

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

Number of signals
Chemical shift
Area under peak
Splitting

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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

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

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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

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

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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)

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

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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

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What is the integration trace?

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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)

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What is TMS (name and structure)?

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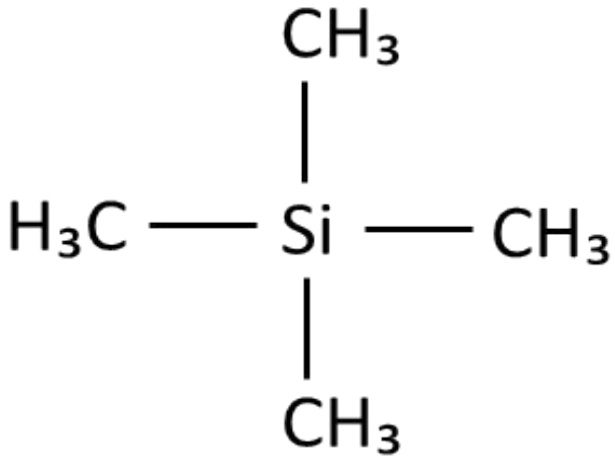
What is TMS (name and structure)?

Tetramethylsilane



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Why is TMS used?

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Why is TMS used?

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

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What are other advantages of using TMS?

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What are other advantages of using TMS?

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

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When does splitting/spin-spin coupling occur?

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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

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What is the n+1 rule?

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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

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

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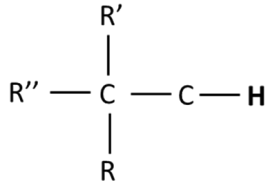
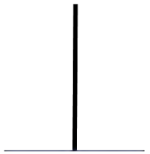
Draw the splitting patterns for 0, 1, 2 and 3 inequivalent H atoms 3 bonds or less away.

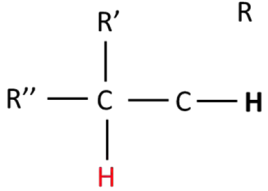
No coupled protons



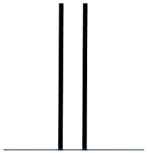
Singlet



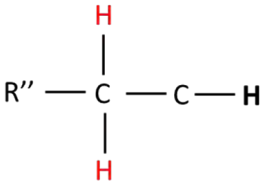
One coupled proton



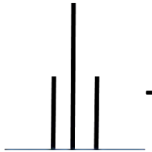
Doublet



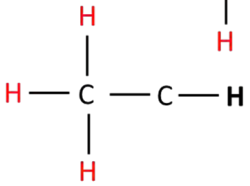
Two coupled protons



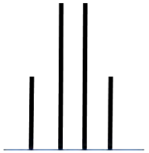
Triplet



Three coupled protons



Quartet



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

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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.

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Which solvents are used?

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Which solvents are used?

Deuterated solvents: $CDCl_3$, D_2O, C_6D_6

CCl_4 - tetrachloromethane

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

Number of signals
Chemical shift
Splitting
Area under peak

CC BY NC ND

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

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

Chemical shift: Larger □ for ^{1}H 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

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

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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.

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