**NMR**

**Nuclear Magnetic Resonance**

**Spectroscopy**

Once you have made a new organic chemical it is important to check that the structure is what you think it should be. The best way of doing this is by running an NMR spectrum.

NMR gives direct information about the chemical environment of hydrogen atoms in molecules. It uses the fact that, in the quantum mechanical sense, the hydrogen atoms are spinning protons and create tiny magnetic fields. They act like small bar magnets (sn). If you put hydrogen atoms in a big external magnetic field (SN), then they line up S:ns:N (a low energy state). By exciting the hydrogen atoms with an oscillating radio signal (another magnetic influence) you can give some of them enough energy to make them flip from the low energy state (S:ns:N) to a high energy state S:sn:N.

When the radio signal is switched off, the protons in the high energy state collapse back to normal, and a discrete amount of energy is given out. This energy is measured as a spectrum.

The magnetic environment of a hydrogen atom is also affected by the electrons in the neighbouring chemical bonds and by other hydrogen atoms in the proximity. Therefore, the position of a peak in the spectrum is dependent upon the chemical environment, and the number of other hydrogen atoms close by. As a bonus, the area under the peak is proportional to the number of hydrogen atoms in a specific environment. This is conveniently measured by the height of the integral line ( ∫ ) over the peak.

NMR spectra are normally calibrated in a scale of parts per million (PPM). The typical positions of various hydrogen atoms are shown below.

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| --- | --- | --- | --- | --- | --- | --- |
| Aromatic |  | 6.5 - 8.0 | Alkene | |  | 4.5 - 5.5 |
|  | | about 2.0 |  | | | 2.5 - 3.5 |
|  | | 3.5 - 4.0 | Alkane |  | | 1.0 - 1.5 |
| N**H** | | variable -often a broad peak | O**H** | | | variable -often a broad peak |

The shape of the signal given by any particular hydrogen atom is related to the number of neighbouring hydrogen atoms on adjacent carbons. Note that this rule does not always apply to hydrogen atoms on oxygen or nitrogen.

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| **Number of neighbouring equivalent hydrogen atoms** | **Shape of signal** |
| 0 | single peak - singlet |
| 1 | two close peaks - doublet |
| 2 | three close peaks - triplet |
| 3 | four close peaks - quartet |

Use your knowledge of NMR to match the following structures with the spectra. Each spectrum is presented as “normal” size plus an expanded version to show finer details.

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| 1 |  | 2 |  |
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| 3 |  | 4 |  |

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| All of the spectra were run using solutions of the compounds in dimethylsulphoxide (DMSO; C2H6SO) which is an excellent solvent for most things.  So that the spectra are not overpowered by MMR signals from |  |

the solvent, the hydrogen atoms in the solvent have been replaced by deuterium (“heavy hydrogen” with one proton and one neutron). NMR signals from deuterium do not show up in normal hydrogen spectra. However, it is very difficult to get DMSO 100% deuterated. There is always a small amount of C2D5HSO in the C2D6SO. The NMR peak due to this residual hydrogen atom is shown in the spectra as “peak due to solvent” at 2.55 on the scale. There is also a trace of water in the DMSO and this is shown as “peak due to solvent” at 3.4 on the scale.

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| graphic3 |

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| graphic6 |

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| graphic7 |

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