Additional higher level

Topic 21: Measurement and analysis

2 hours

Essential idea: Although spectroscopic characterization techniques form the backbone of structural identification of compounds, typically no one technique results in a full structural identification of a molecule.

21.1 Spectroscopic identification of organic compounds

Nature of science:

Improvements in modern instrumentation—advances in spectroscopic techniques (IR, ^{1}H NMR and MS) have resulted in detailed knowledge of the structure of compounds. (1.8)

Understandings:

- Structural identification of compounds involves several different analytical techniques including IR, ^{1}H NMR and MS.
- In a high resolution ^{1}H NMR spectrum, single peaks present in low resolution can split into further clusters of peaks.
- The structural technique of single crystal X-ray crystallography can be used to identify the bond lengths and bond angles of crystalline compounds.

Applications and skills:

- Explanation of the use of tetramethylsilane (TMS) as the reference standard.
- Deduction of the structure of a compound given information from a range of analytical characterization techniques (X-ray crystallography, IR, ^{1}H NMR and MS).

Guidance:

- Students should be able to interpret the following from ^{1}H NMR spectra: number of peaks, area under each peak, chemical shift and splitting patterns. Treatment of spin-spin coupling constants will not be assessed but students should be familiar with singlets, doublets, triplets and quartets.
- High resolution ^{1}H NMR should be covered.

International-mindedness:

- The chemical community often shares chemical structural information on the international stage. The Cambridge Crystallographic Database, ChemSpider developed by the *Royal Society of Chemistry* and the *Protein Data Bank (RCSB PDB)* (at Brookhaven National Laboratory, USA) are examples which highlight the international nature of the scientific community.

Theory of knowledge:

- The intensity ratio of the lines in the high resolution NMR spectrum is given by the numbers in Pascal's triangle, a mathematical pattern known independently over a thousand years ago by a number of different cultures. Why is mathematics such an effective tool in science? Is mathematics the science of patterns?

Utilization:

- Protons in water molecules within human cells can be detected by magnetic resonance imaging (MRI), giving a three-dimensional view of organs in the human body. Why is MRI replacing computerized tomography (CT) scans for some applications but is used as a complementary technique for others?
- MS (and other techniques such as TLC, GC, GC-MS and HPLC) can be used in forensic investigations at crime scenes.
- Analytical techniques can be used to test for drug abuse by high-performance athletes.

21.1 Spectroscopic identification of organic compounds	
• The precise details of single crystal X-ray crystallography need not be known in detail, but students should be aware of the existence of this structural technique in the wider context of structural identification of both inorganic and organic compounds. • The operating principles are not required for any of these methods.	Syllabus and cross-curricular links: Topic 11.3—spectroscopic identification of compounds Option B.2—chromatography and protein separation Option B.9—chromatography and pigments Option D.7—chiral auxiliaries **Aims:** • **Aim 7**: Spectral databases can be used here.