21. Measurement and analysis (HL)

Syllabus:

21.1 Spectroscopic identification of organic compounds

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.

21.1 Spectroscopic identification of organic compounds

(A) Further NMR spectroscopy

There are 12 H nuclei which are in the same environment in TMS molecule, and NMR signals are measured against a standard produced by them.

In low-resolution ^{1}H NMR, there are several single peaks.

But in high-resolution ^{1}H NMR, the peaks are not only just single peaks, some may split into a group of smaller parts.

The splitting is due to the spin – spin coupling, that depends on the number of adjacent protons.

Three key things for the high-resolution ^{1}H NMR,

- Protons bonded to the same atom do not interact with one another as they are equivalent and behave as a group
- Protons on non-adjacent carbon atoms do not generally interact with one another
- The O–H single peak in ethanol does not split.

Numbers of adjacent proton (n)	Number of split (n + 1)	Pascal pattern	Splitting pattern
0	1	1	Singlet
1	2	1 1	Doublet
2	3	1 2 1	Triplet
3	4	1 3 3 1	Quartet
4	5	1 4 6 4 1	Quintet
5	6	1 5 10 10 5 1	Sextet