# 3.3.15 NMR Spectroscopy



**★ A-LEVEL ONLY — not examined at AS level**

| 3.3.15 | *NMR spectroscopy: 13C and 1H NMR. Chemical shift. Integration. (n+1) rule. TMS. Deuterated solvents.* |
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13C NMR: number of peaks = number of different carbon environments. Simpler spectra than 1H (no splitting shown).

1H NMR: number of peaks = number of different proton environments. Peak area (integration) = relative number of H atoms.

(n+1) rule: a peak is split into n+1 lines by n adjacent non-equivalent H atoms. Singlet (0 neighbours), doublet (1), triplet (2), quartet (3).

Chemical shift (delta, in ppm): position of peak. Depends on molecular environment — use AQA data booklet.

TMS (tetramethylsilane, Si(CH3)4): reference standard (delta = 0). Chosen because: 12 equivalent H atoms (one sharp peak), delta = 0 away from most signals, inert, volatile, miscible with most organic solvents.

Deuterated solvents (e.g. CDCl3): D (2H) is NMR-inactive → no interfering peaks from solvent.

D2O shake: O–H and N–H peaks disappear (H exchanged for D) → confirms OH or NH present.