M.Sc. Semester-III
Core Course - 7 (CC-7)
Application of Spectroscopy

III. Nuclear Magnetic Resonance Spectroscopy

L1: Basic Principle of PMR Spectroscopy

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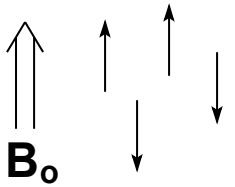
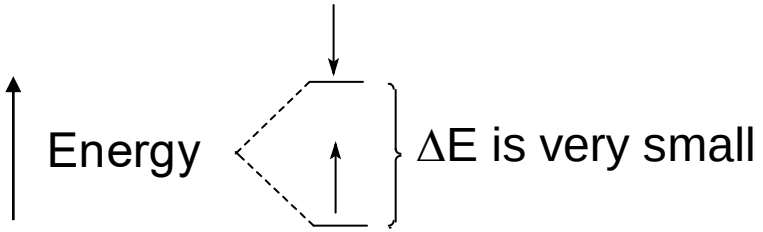
Basic Principle : Theory of NMR

- The positively charged nuclei of certain elements (e.g., ^{13}C and ^{1}H) behave as tiny magnets.

- In the presence of a strong external magnetic field (B_o), these nuclear magnets align either with (↑) the applied field or opposed to (↓) the applied field.

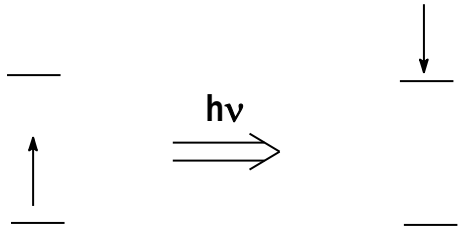


- The latter (opposed) is slightly higher in energy than aligned with the field.



Theory of NMR

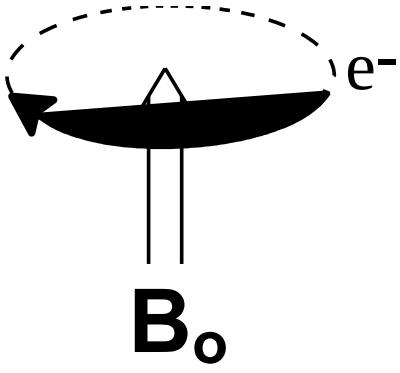
- The small energy difference between the two alignments of magnetic spin corresponds to the energy of radio waves according to Einstein's equation $E=h\nu$.



- Application of just the right radiofrequency (ν) causes the nucleus to "flip" to the higher energy spin state
- Not all nuclei require the same amount of energy for the quantized spin 'flip' to take place.
- The exact amount of energy required depends on the chemical identity (H, C, or other element) and the chemical environment of the particular nucleus.

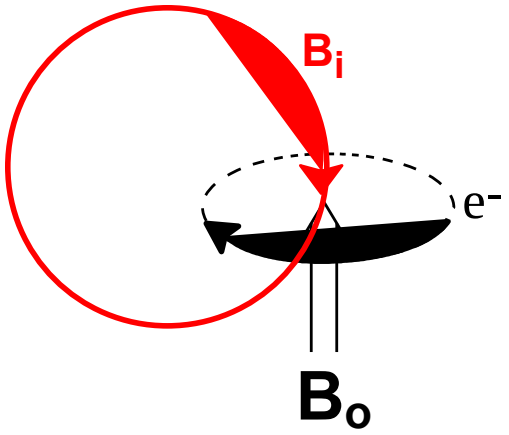
Theory of NMR

- Nuclei are surrounded by electrons. The strong applied magnetic field (B_o) induces the electrons to circulate around the nucleus (left hand rule).



Theory of NMR

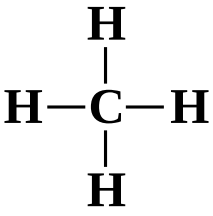
- The induced circulation of electrons sets up a secondary (induced) magnetic field (B_i) that **<u>opposes</u>** the applied field (B_o) at the nucleus (right hand rule).

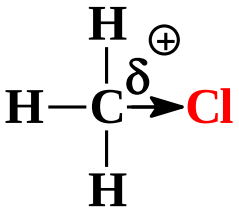


- We say that nuclei are **<u>shielded</u>** from the full applied magnetic field by the surrounding electrons because the secondary field diminishes the field at the nuclei.

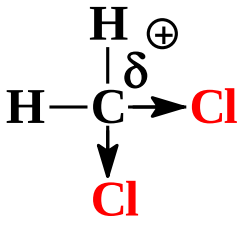
Theory of NMR

- The electron density surrounding a given nucleus depends on the **electronegativity** of the attached atoms.
- The more electronegative the attached atoms, the less the electron density around the nucleus in question.
- We say that that nucleus is less shielded, or is **deshielded** by the electronegative atoms.
- **Deshielding** effects are generally additive. That is, two highly electronegative atoms (2 Cl atoms, for example) would cause more deshielding than only 1 Cl atom.



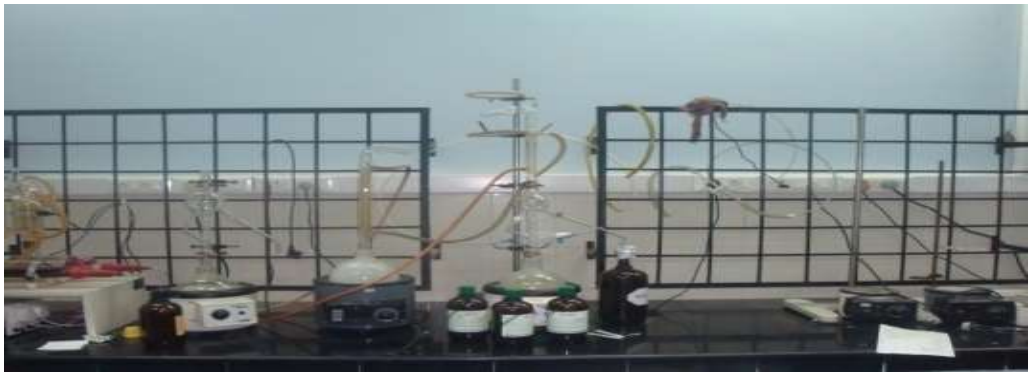


C and H are deshielded



C and H are more deshielded

Thank You



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