Nuclear Magnetic Resonance Spectroscopy

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SIMPLE PLAN ! THAT'S SO SIMPLE

1.Principles of molecular spectroscopy

2. Nuclear Shieldingand^{1}H Chemical Shifts

Lets understand few things

- Electromagnetic Radiation –

is propagated at the speed of light

has properties of particles and waves

the energy of a photon is proportional to its frequency

the Electromagnetic spectrum

Shorter Wavelength (λ)

Longer Wavelength (λ)

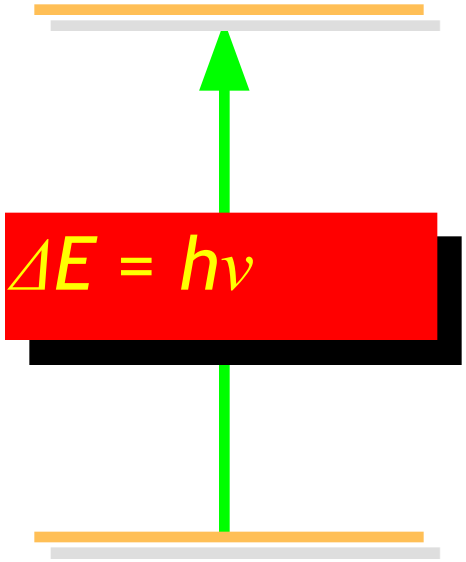
Higher Frequency (ν)

Lower Frequency (ν)

Higher Energy (E)

Lower Energy (E)

1. Principles



- Electromagnetic radiation is absorbed when the energy of photon corresponds to difference in energy between two states.

What Kind of States?

electronic	UV-Vis
vibrational	infrared
rotational	microwave
nuclear spin	radiofrequency

The nuclei that are most useful to organic chemists are:

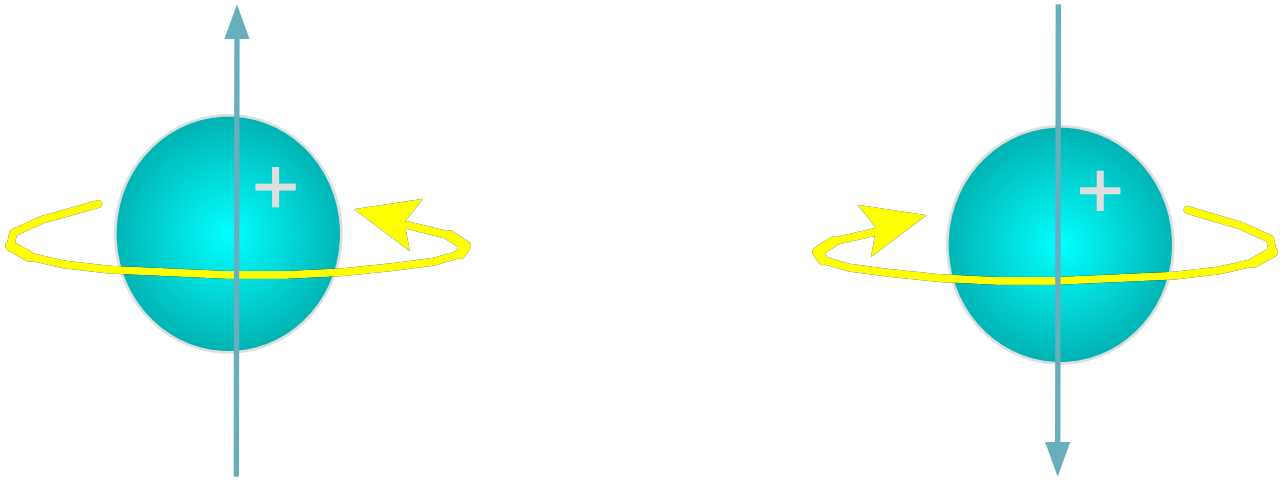
^{1}H and ^{13}C

both have spin = ±1/2

^{1}H is 99% at natural abundance

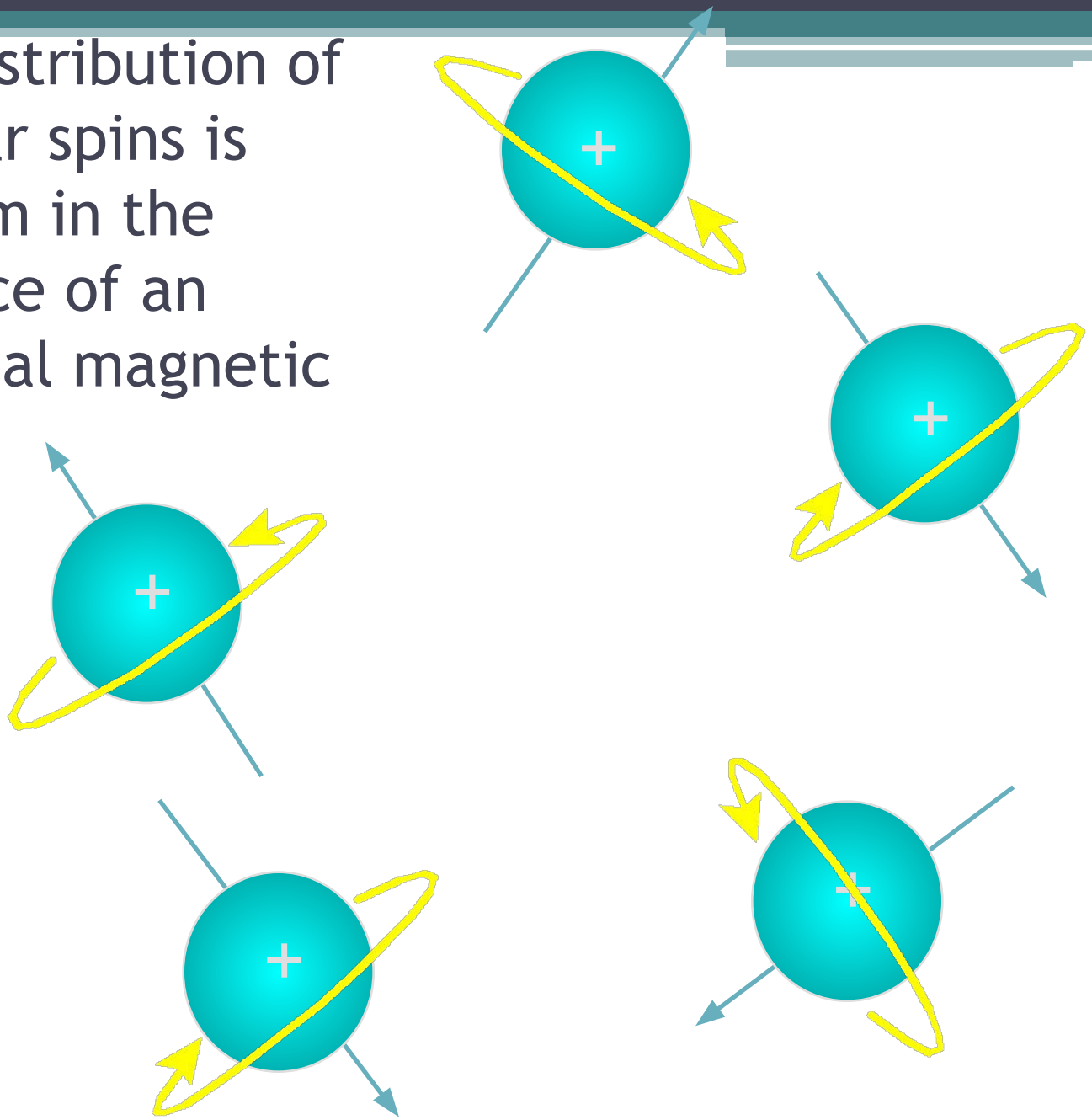
^{13}C is 1.1% at natural abundance

Nuclear Spin

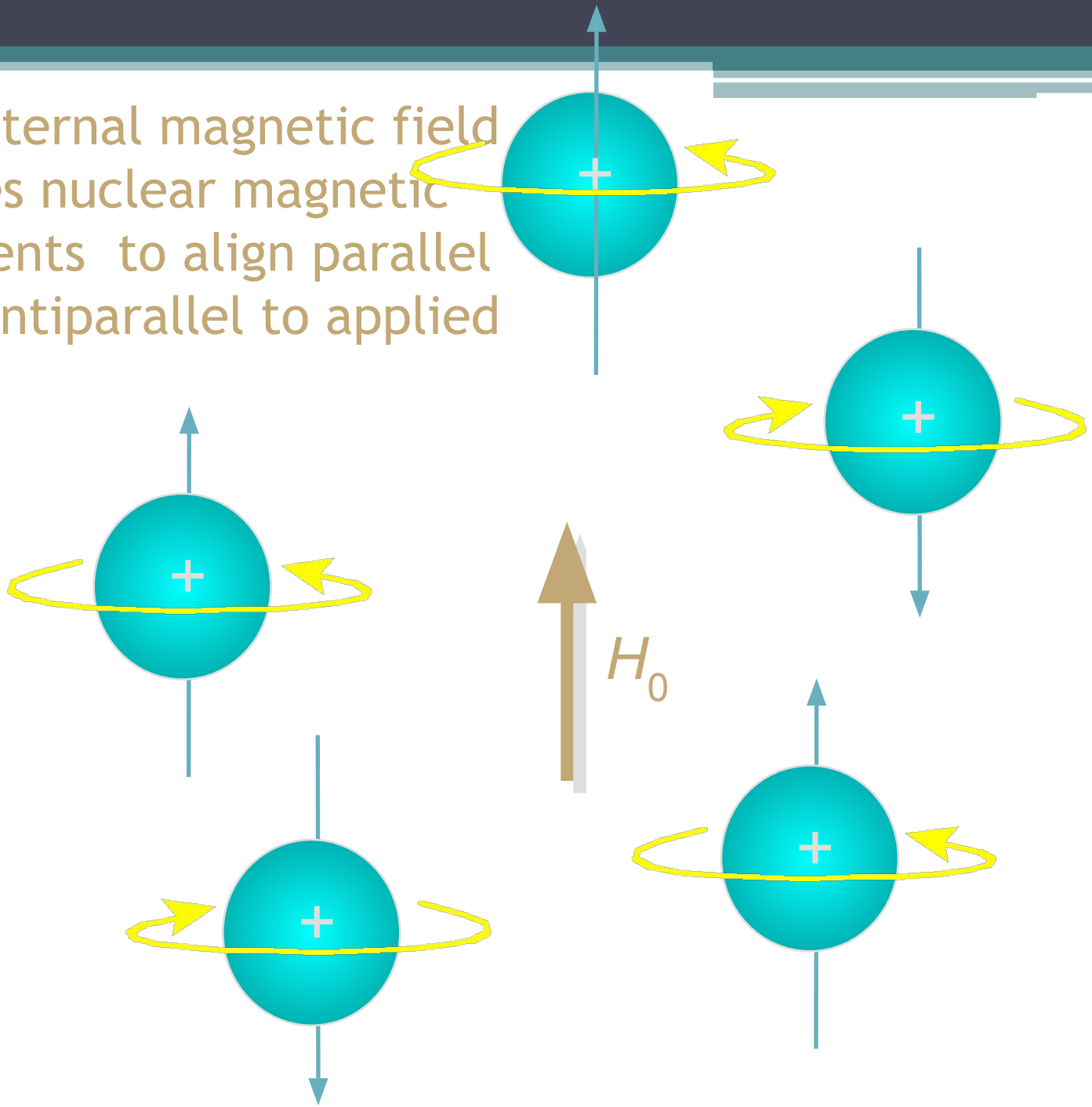


A spinning charge, such as the nucleus of ^{1}H or ^{13}C, generates a magnetic field. The magnetic field generated by a nucleus of spin +1/2 is opposite in direction from that generated by a nucleus of spin –1/2.

The distribution of nuclear spins is random in the absence of an external magnetic field.



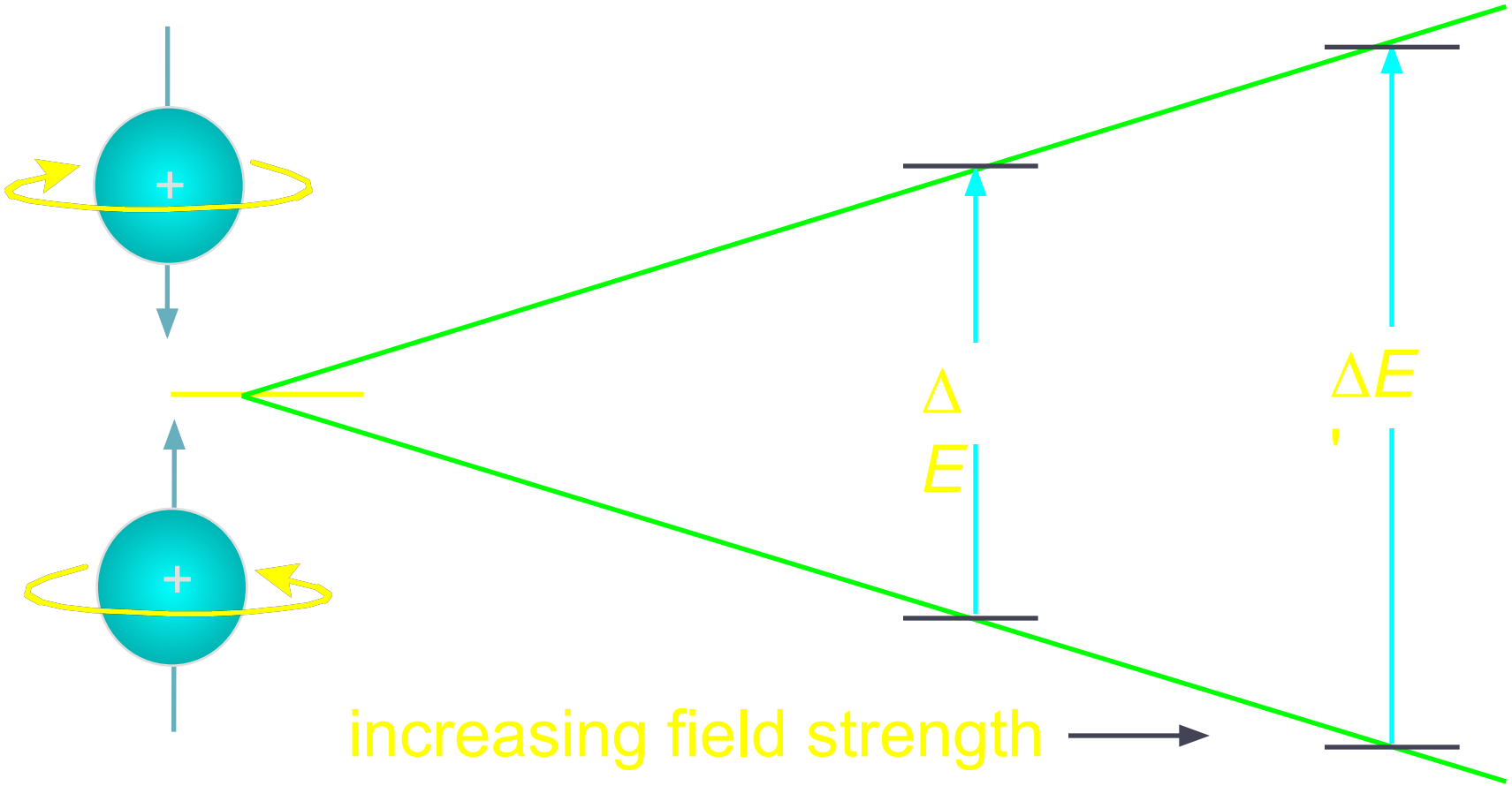
An external magnetic field causes nuclear magnetic moments to align parallel and antiparallel to applied field.



Some important relationships in NMR

	Units
The frequency of absorbed electromagnetic radiation is proportional to	Hz
the energy difference between two nuclear spin states which is proportional to	kJ/mol (kcal/mol)
the applied magnetic field	tesla (T)

Energy Differences Between Nuclear Spin States



no difference in absence of magnetic field

proportional to strength of external magnetic field

- The frequency of absorbed electromagnetic radiation for a particular nucleus (such as ^{1}H) depends on its molecular environment.

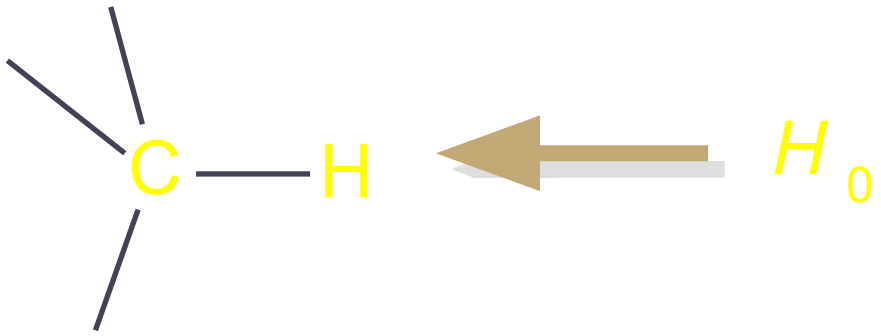
  This is why NMR is such a useful tool for structure determination.

2. Nuclear Shielding

What do we mean by "shielding?"

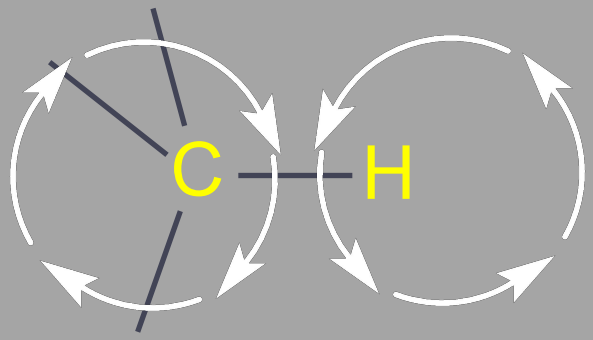
What do we mean by "chemical shift?"

- An external magnetic field affects the motion of the electrons in a molecule, inducing a magnetic field within the molecule.



An external magnetic field affects the motion of the electrons in a molecule, inducing a magnetic field within the molecule.

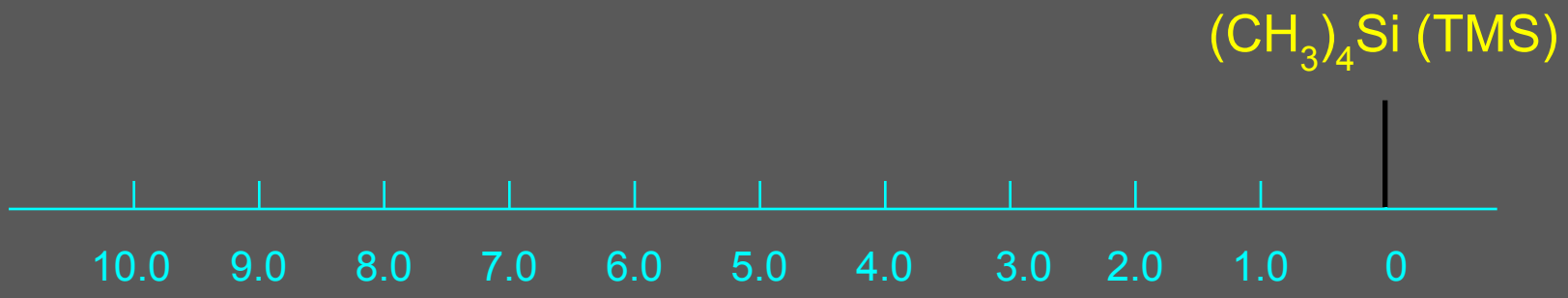
The direction of the induced magnetic field is opposite to that of the applied field.



- The induced field shields the nuclei (in this case, C and H) from the applied field.
  - A stronger external field is needed in order for energy difference between spin states to match energy of rf radiation.
- Chemical shift is a measure of the degree to which a nucleus in a molecule is shielded.
  - Protons in different environments are shielded to greater or lesser degrees; they have different chemical shifts.

Downfield
Decreased shielding

Upfield
Increased shielding



Chemical shift (δ, ppm)
measured relative to TMS

Effects of Molecular Structure on ^1H Chemical Shifts

- protons in different environments experience different degrees of shielding and have different chemical shifts

$CHCl_3$ δ 7.3 ppm

CH_2Cl_2 δ 5.3 ppm

CH_3Cl δ 3.1 ppm

CH_3F δ 4.3 ppm *least shielded H*

CH_3OCH_3 δ 3.2 ppm

$CH_3N(CH_3)_2$ δ 2.2 ppm

CH_3CH_3 δ 0.9 ppm

$CH_3Si(CH_3)_3$ δ 0.0 ppm *most shielded H*

Conclusion

- A spinning charge can make us understand the structure of matter
- An external magnetic field affects the motion of the electrons in a molecule
- NMR useful tool for structure determination.

THIS IS THE END. THX FOR ATTENTION.