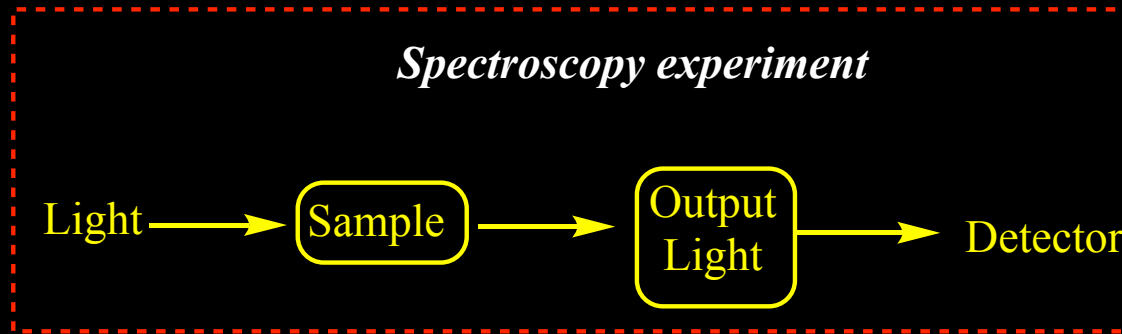
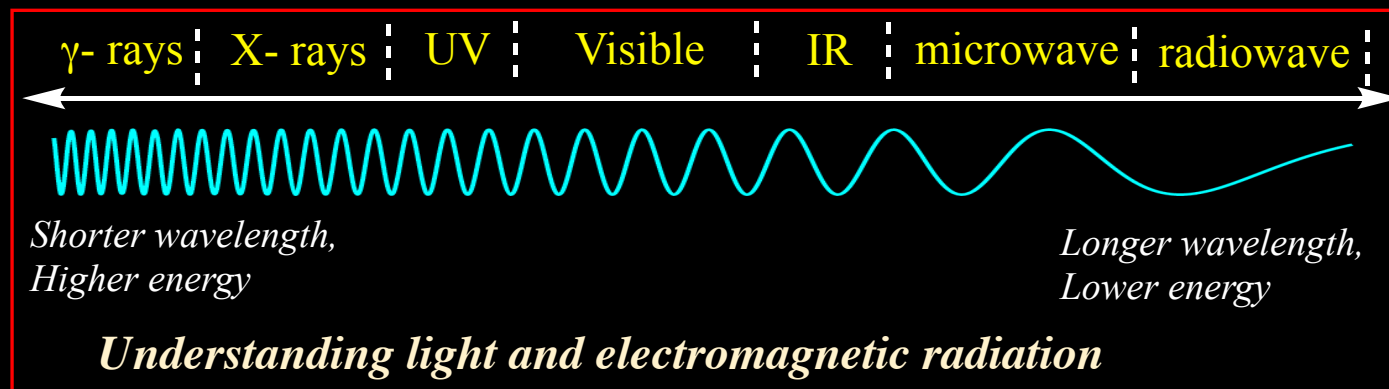


Spectroscopy

Spectroscopy is the study of the interaction between matter and electromagnetic radiation as a function of the wavelength or frequency of the radiation



Spectroscopy



★ UV-Spectroscopy:

Studies the changes in the electronic energy levels within the molecule arising due to transfer of electrons from π or non-bonding electrons

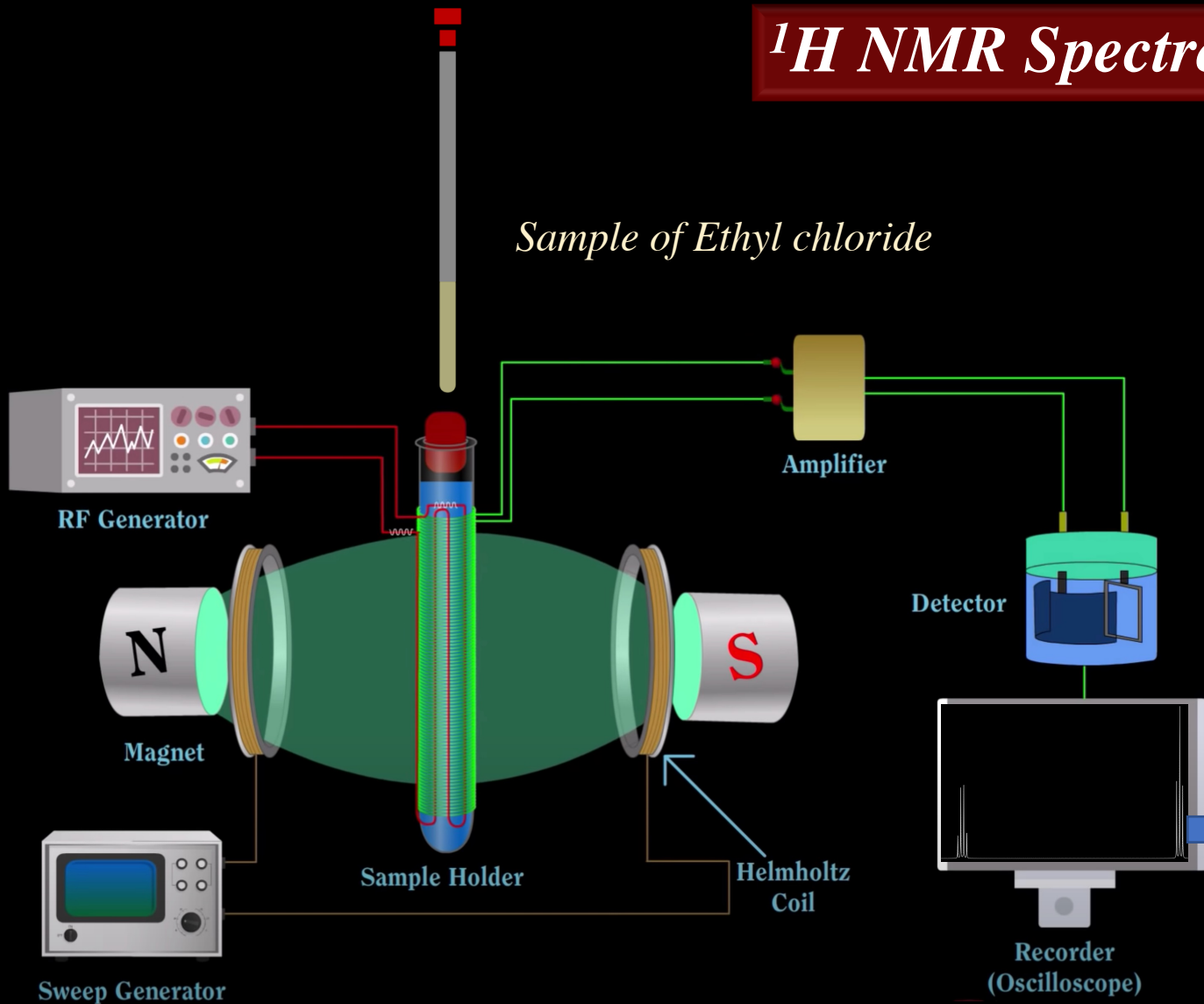
★ IR-Spectroscopy:

Studies the changes in the vibrational and rotational movements of the molecule

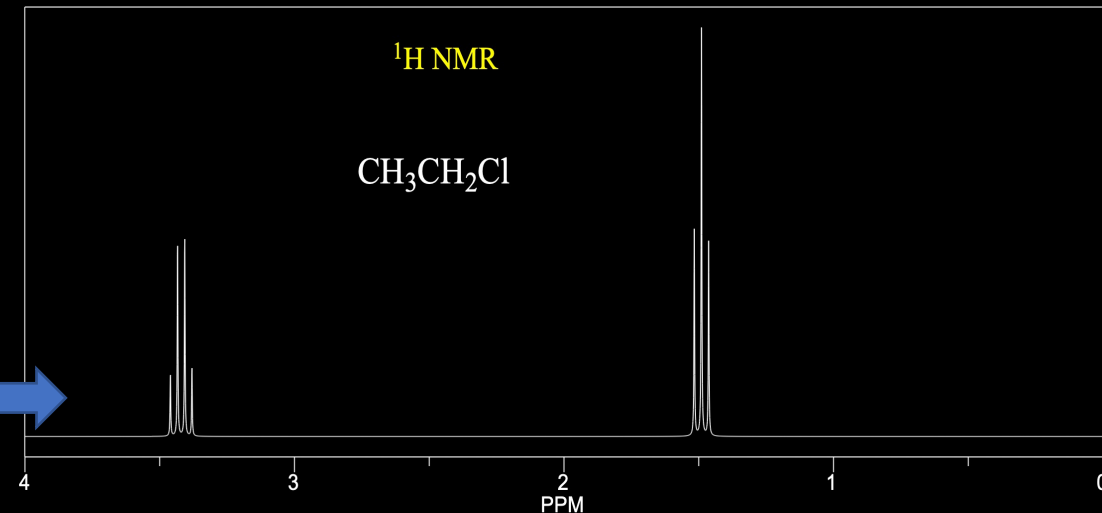
★ NMR-Spectroscopy:

Provides the information about changes in magnetic properties of certain atomic nuclei (eg: ^1H and ^{13}C).

^1H NMR Spectroscopy



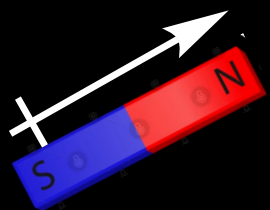
Question: How can we identify ethyl chloride from this graph (spectra)?



^1H NMR Spectra ethyl chloride

NMR Instrumentation

☆ Principle:



Magnet

^1H NMR Spectroscopy

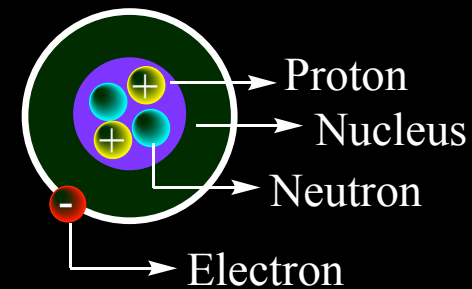
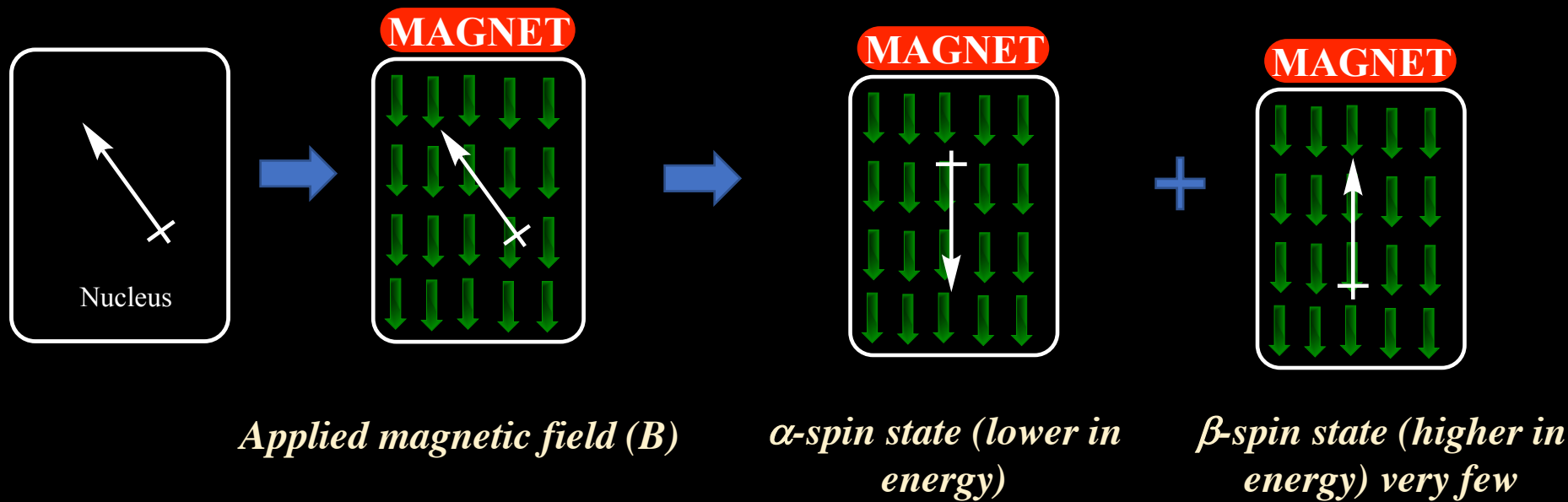
^1H , ^{13}C , ^{15}N , ^{19}F , ^{31}P

*Odd number of protons (or) Odd number of Neutrons
(or) Both*



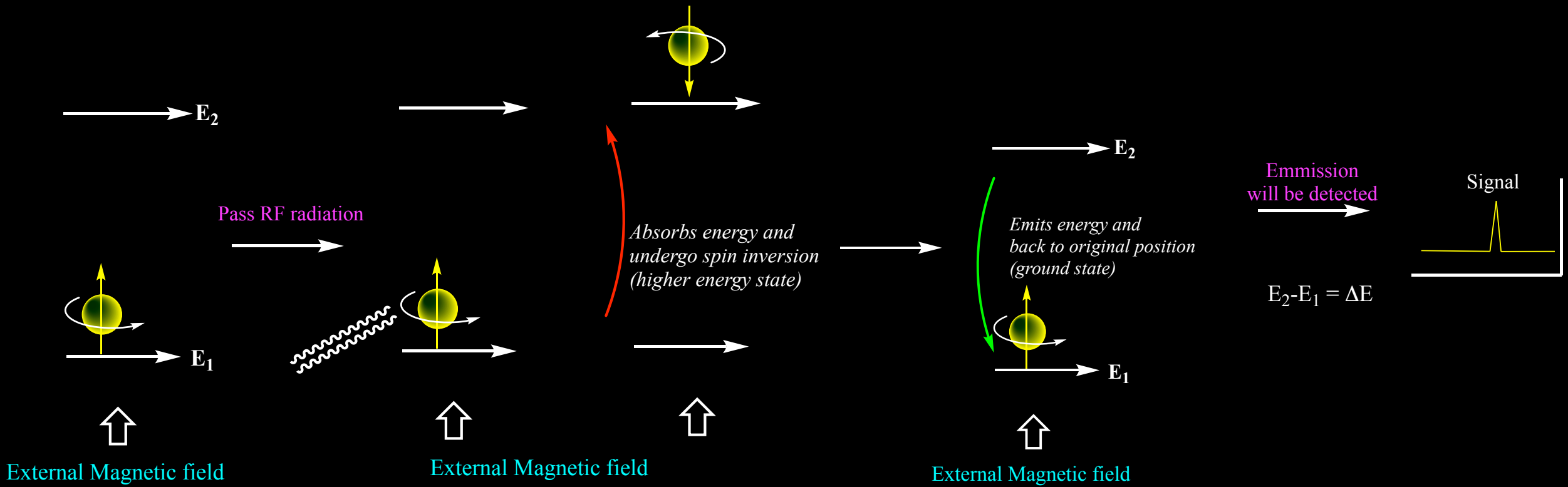
Align in one direction

☆ Basic concept:



The nucleus has a positive charge and is spinning. This generates a small magnetic field. This nucleus behave like a tiny magnet

^1H NMR Spectroscopy



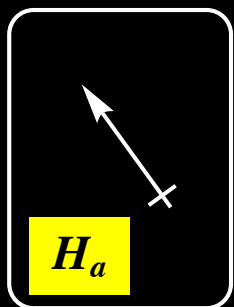
★ How different signal arises?

^1H NMR Spectroscopy

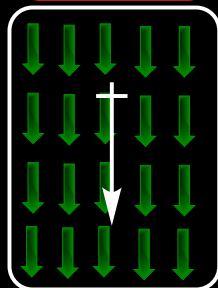
Just assume that we are analyzing two different kind of H atoms H_a and H_b

★ Case-1:

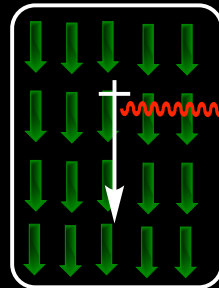
MAGNET



MAGNET



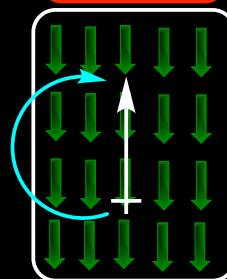
MAGNET



α to β
Spin state



MAGNET



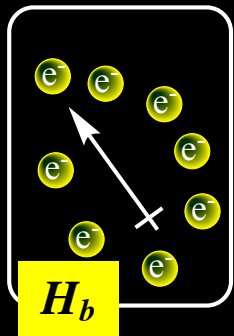
External
magnetic field

Pass RF light

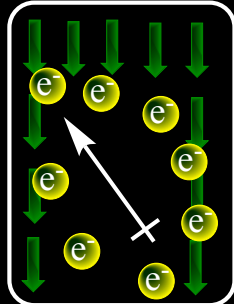
Requires more energy (E_1)

★ Case-2:

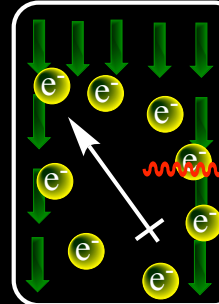
MAGNET



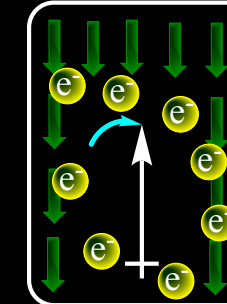
MAGNET



MAGNET



MAGNET

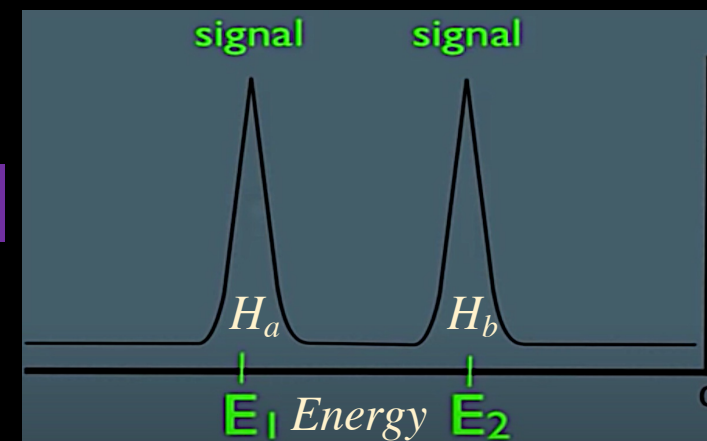


Pass RF light

Requires less energy (E_2)

★ H_a is deshielded

Requires more energy (E_1)



★ H_b is shielded

Requires less energy (E_2)

Surrounded by
electrons

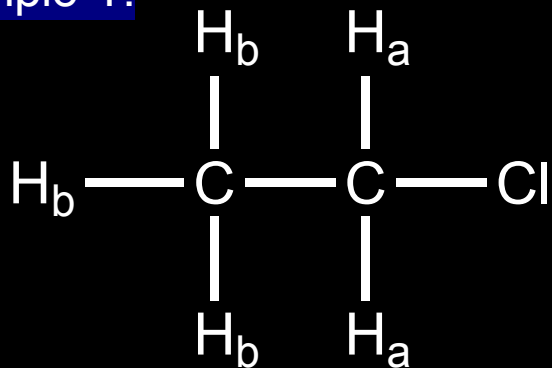
Diamagnetic
Shielding

★ Examples:

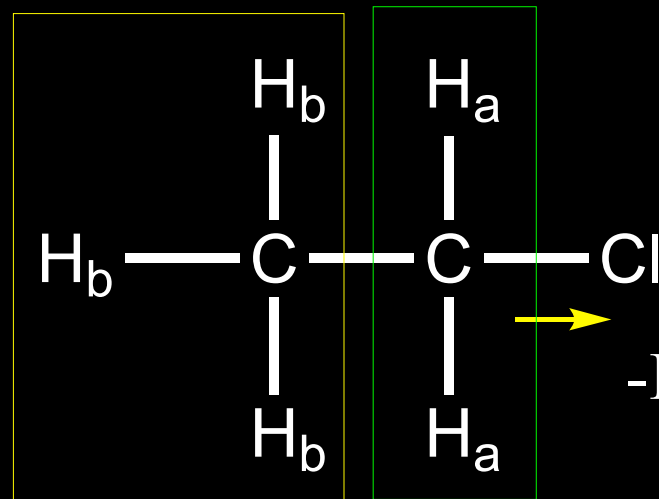
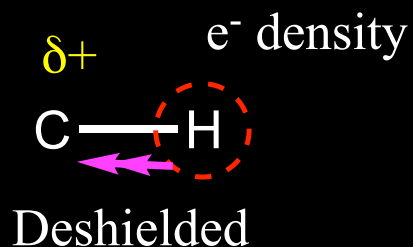
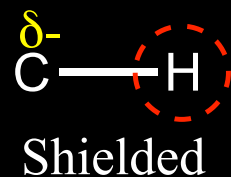


^1H NMR Spectroscopy

★ Example-1:

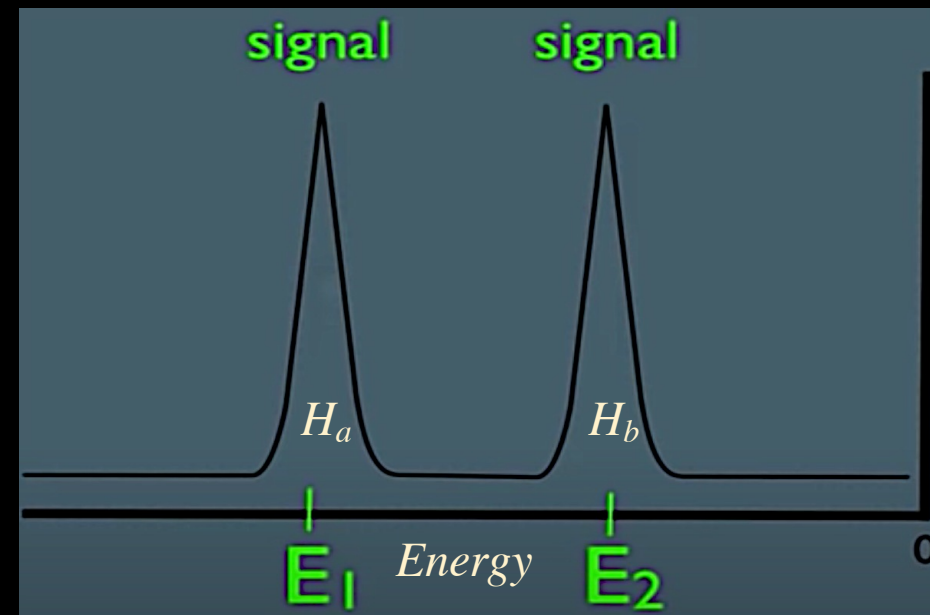


H_a and H_b are chemically non-equivalent



shielded
(Lower energy)

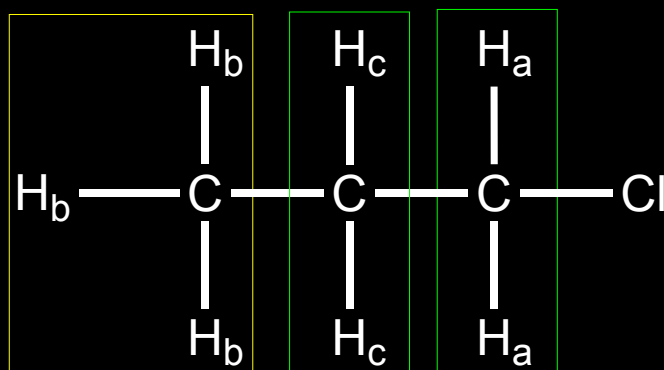
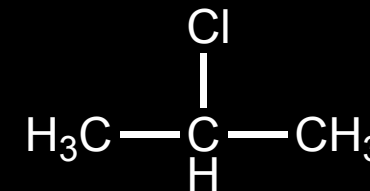
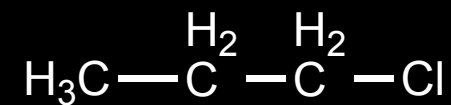
Deshielded
(higher energy)



★ Example-2:

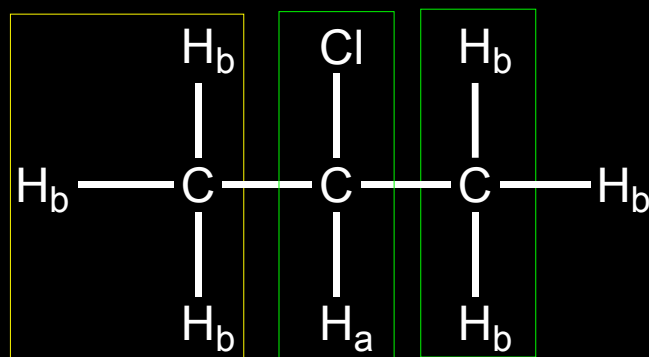
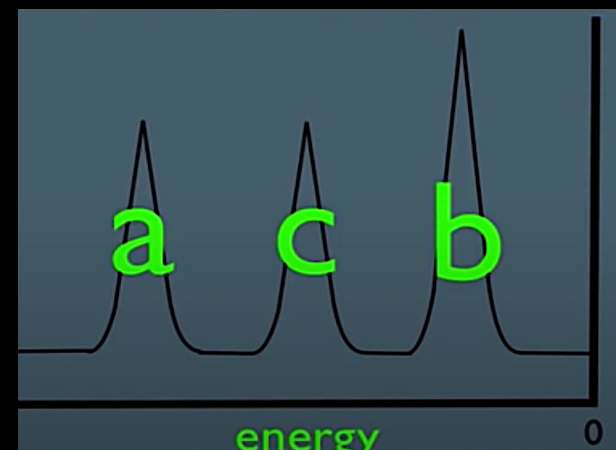
¹H NMR Spectroscopy

• $\text{C}_3\text{H}_7\text{Cl}$



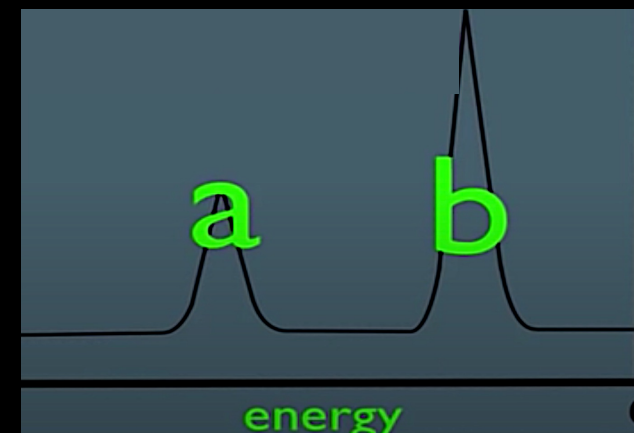
most shielded
(Lower energy)

most Deshielded
(higher energy)



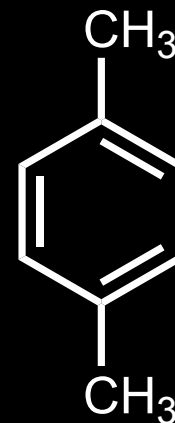
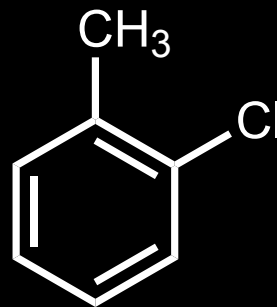
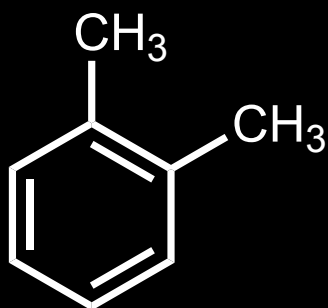
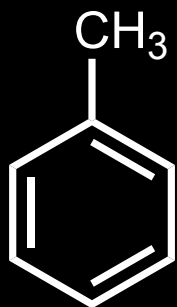
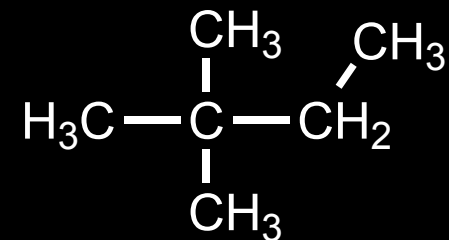
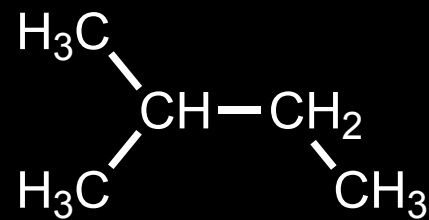
shielded
(Lower energy)

Deshielded
(higher energy)



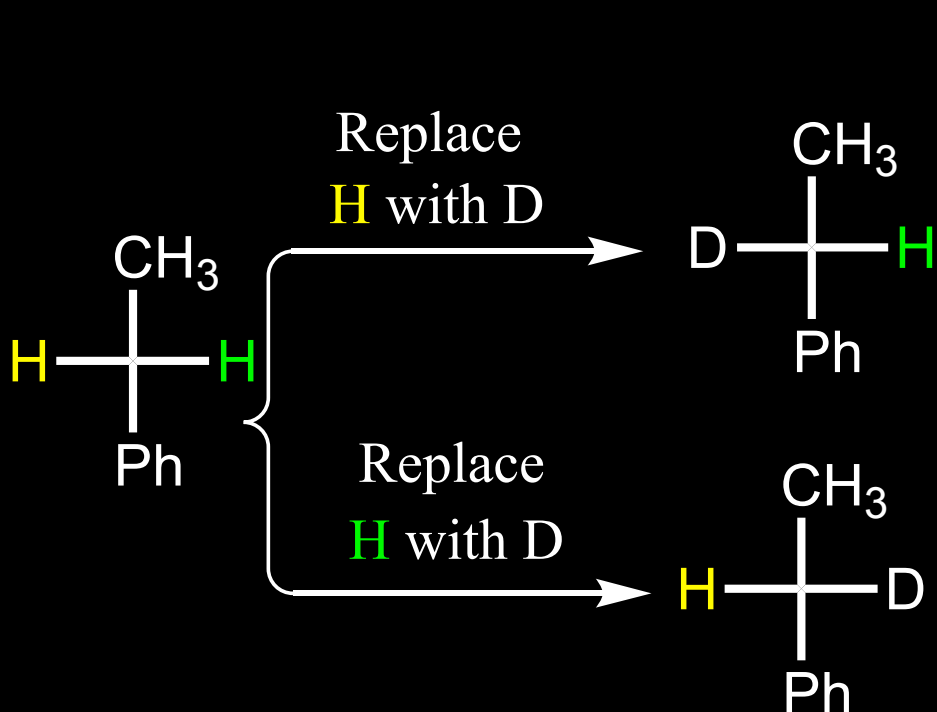
¹H NMR Spectroscopy

How many signals would appear in ¹H NMR for the following molecules?

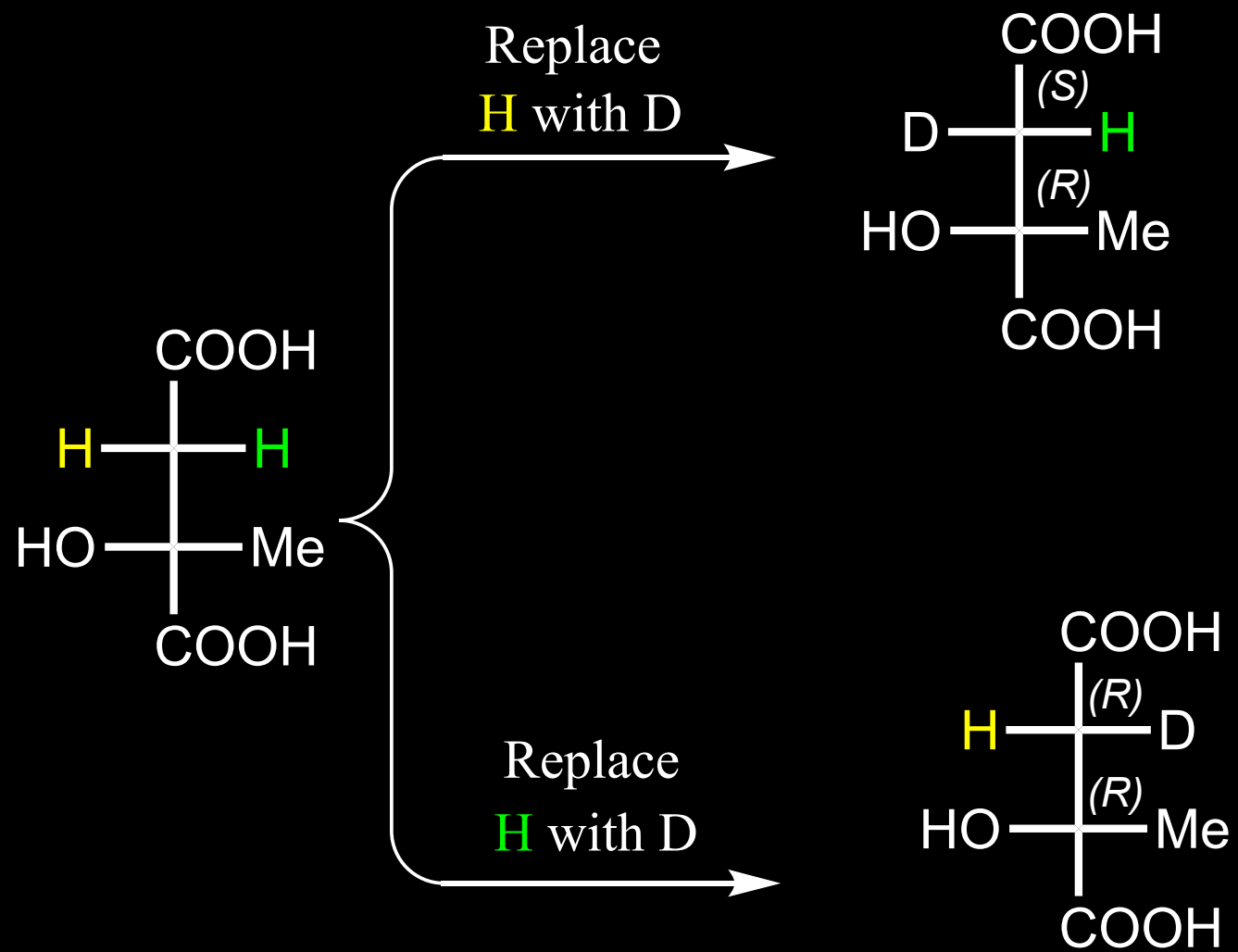


¹H NMR Spectroscopy

Topicity



- Both are Enantiomers
H and H are Enantiotopic



- Both are Diastereomers
H and H are Diastereotopic

How many signals would appear in ¹H NMR for the following molecules?

