
NMR Spectroscopy of Organic Compounds

Lesson 7:
Fluorine, phosphorus, nitrogen, ...



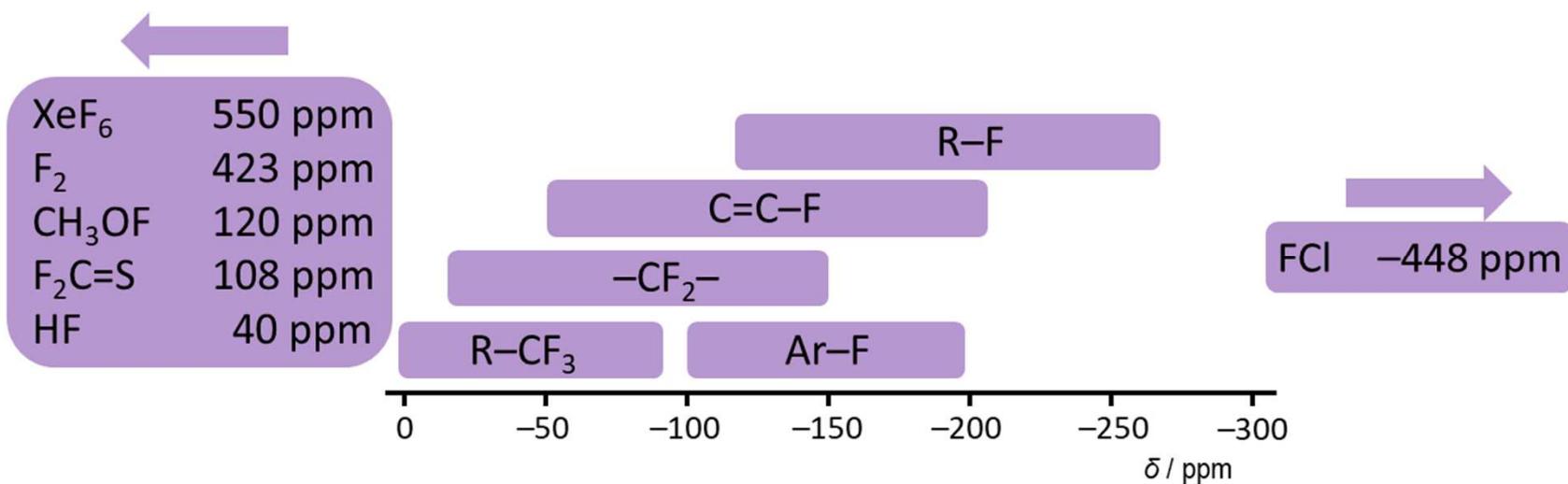
Martin Dračínský

Overview

- ^{19}F , ^{31}P , ^{15}N , ^2H , ^3H

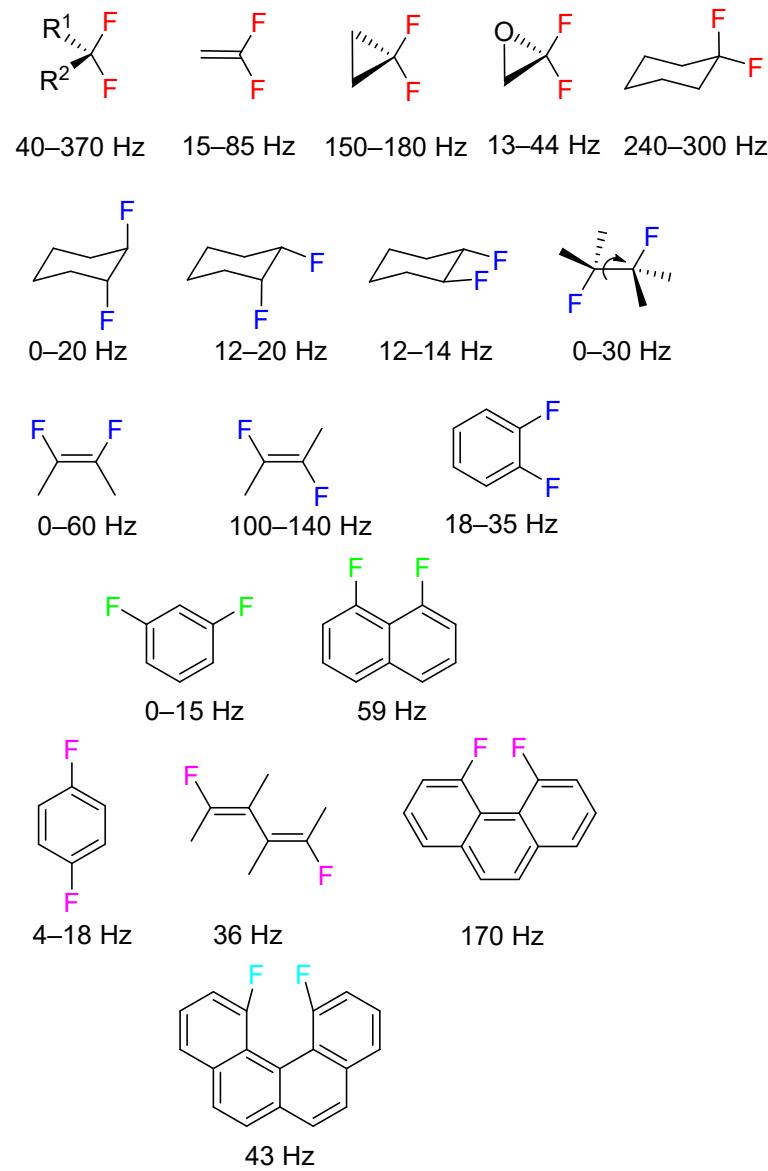
Fluorine ^{19}F

- 100% natural abundance
- High gyromagnetic ratio (470 MHz on a 500MHz spectrometer)
- High sensitivity
- Large span of chemical shifts

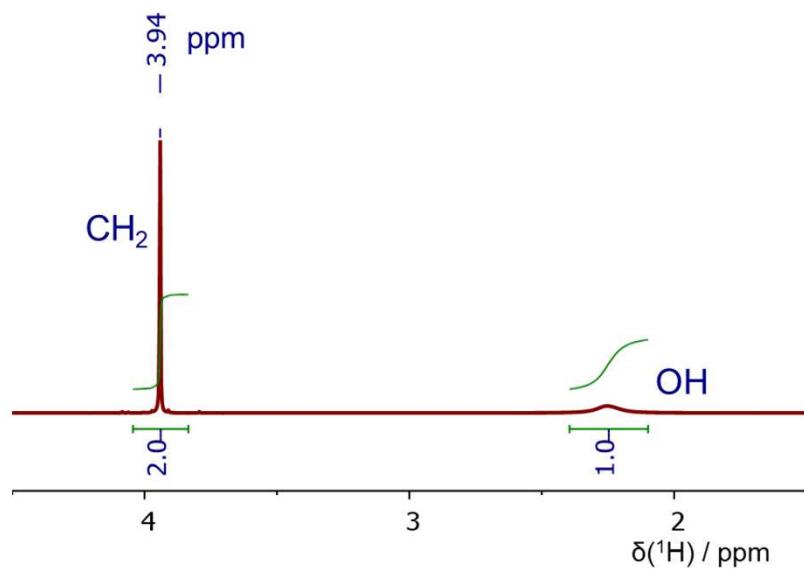
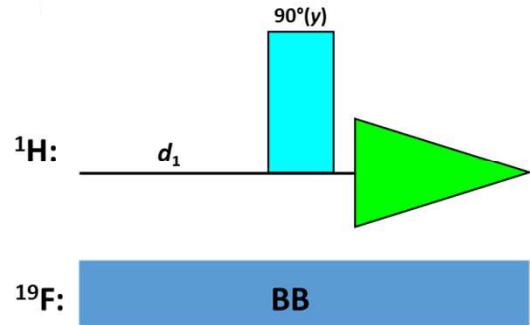
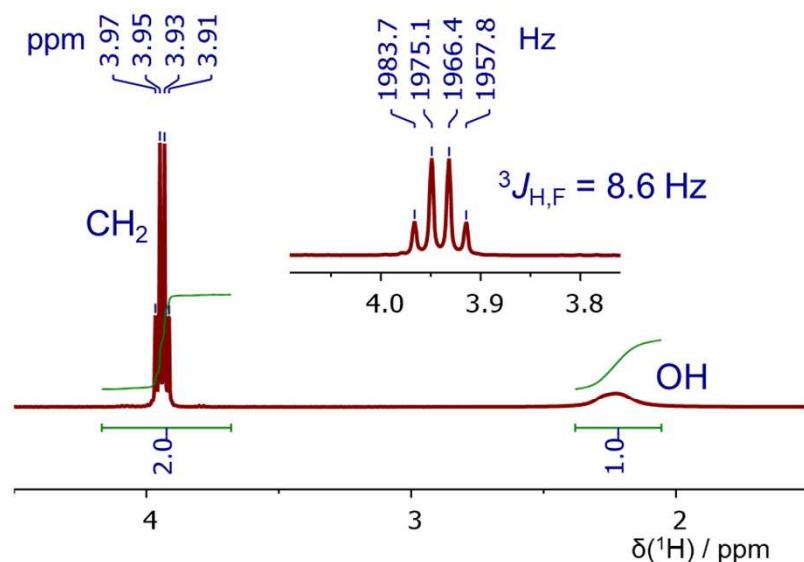
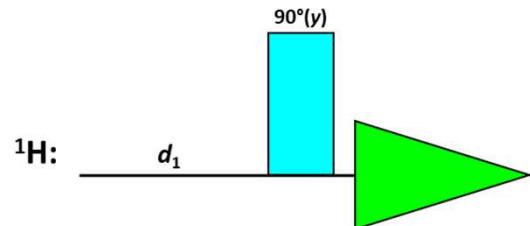


Fluorine ^{19}F

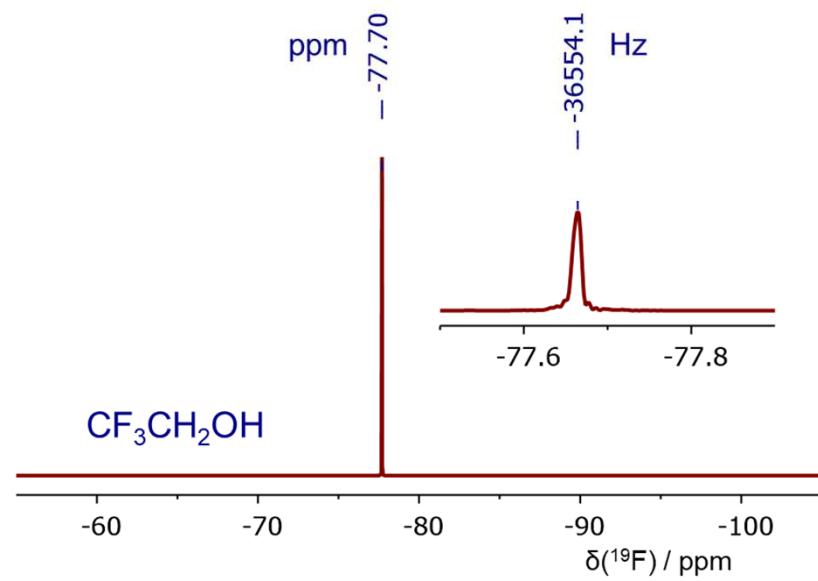
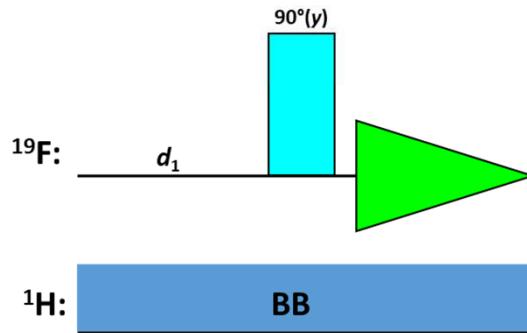
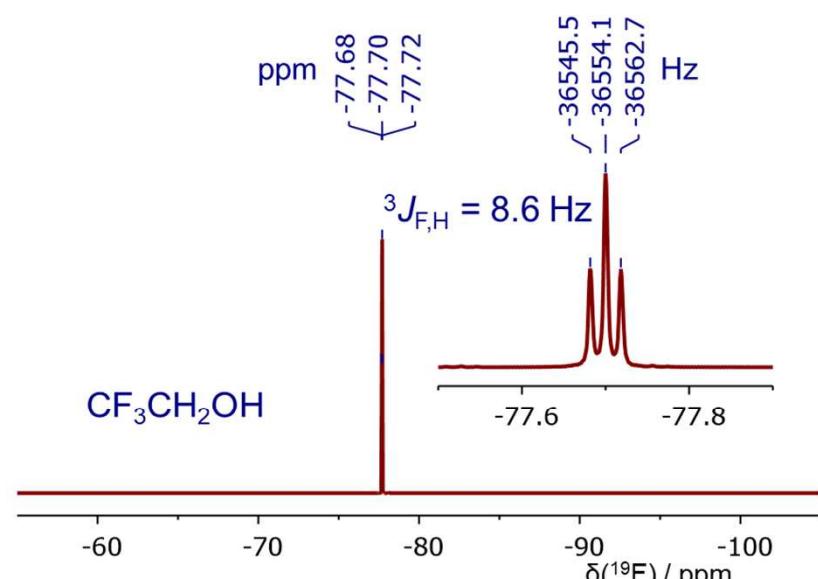
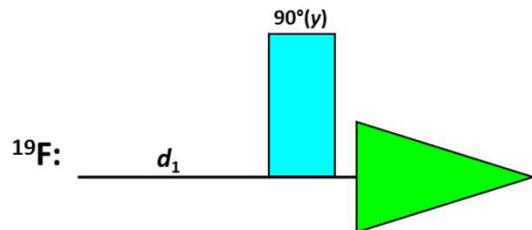
- F,F coupling
- Spatial proximity plays a role



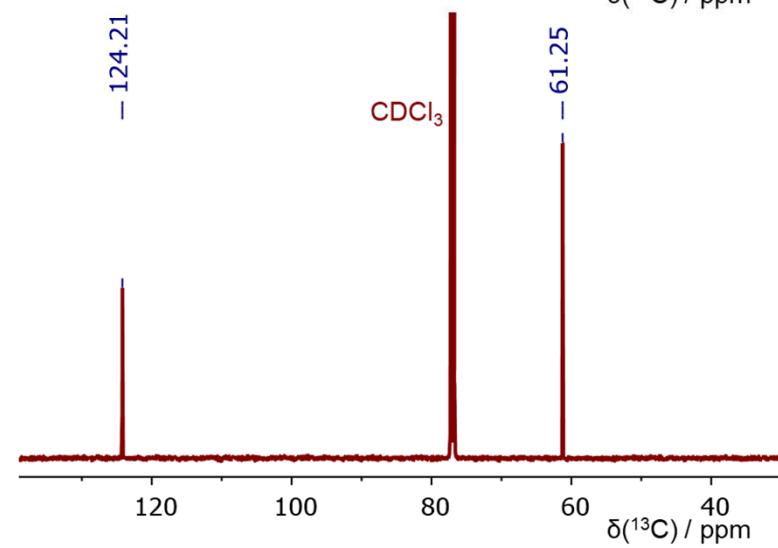
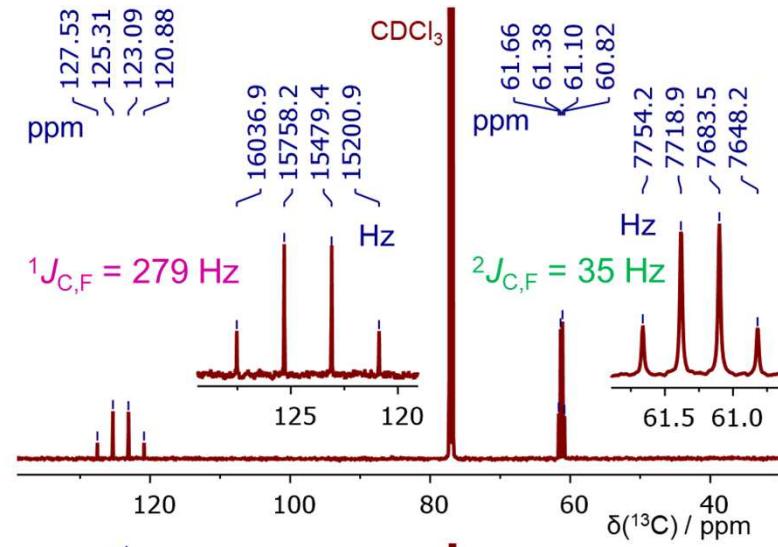
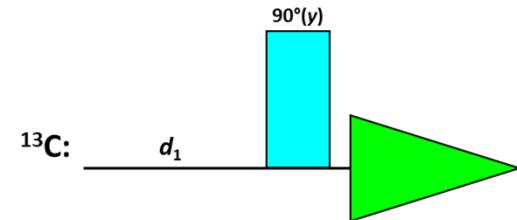
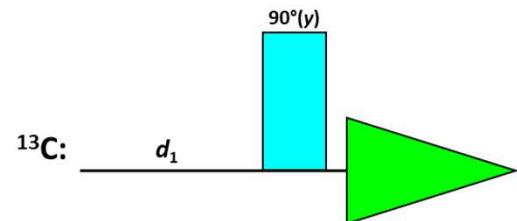
$\text{CF}_3\text{CH}_2\text{OH}$



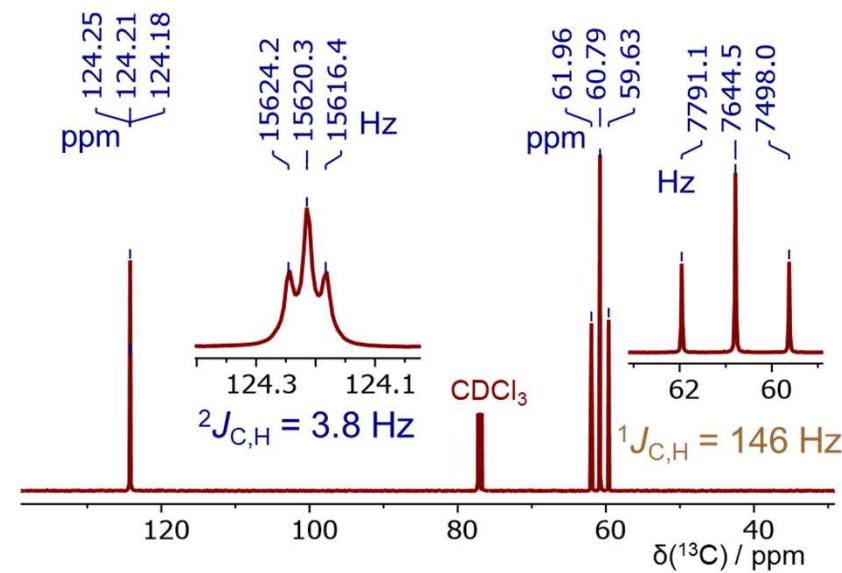
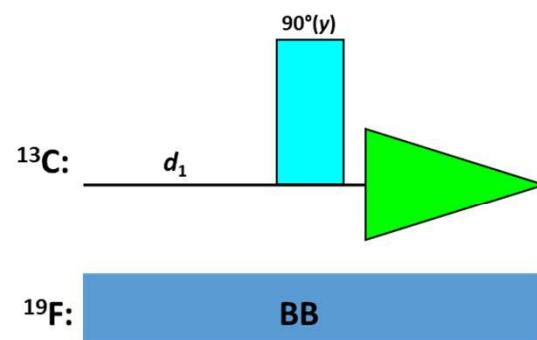
$\text{CF}_3\text{CH}_2\text{OH}$



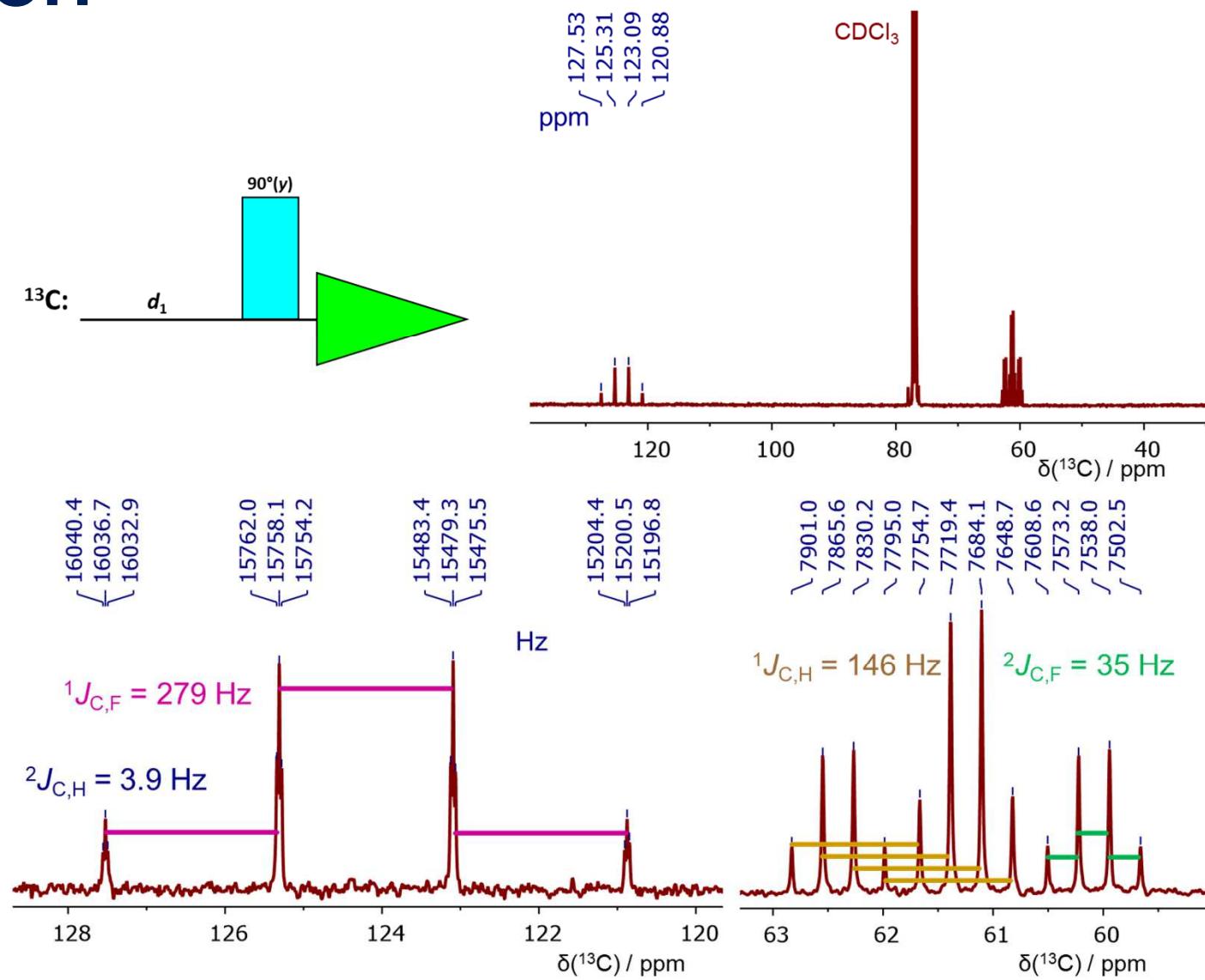
$\text{CF}_3\text{CH}_2\text{OH}$



$\text{CF}_3\text{CH}_2\text{OH}$

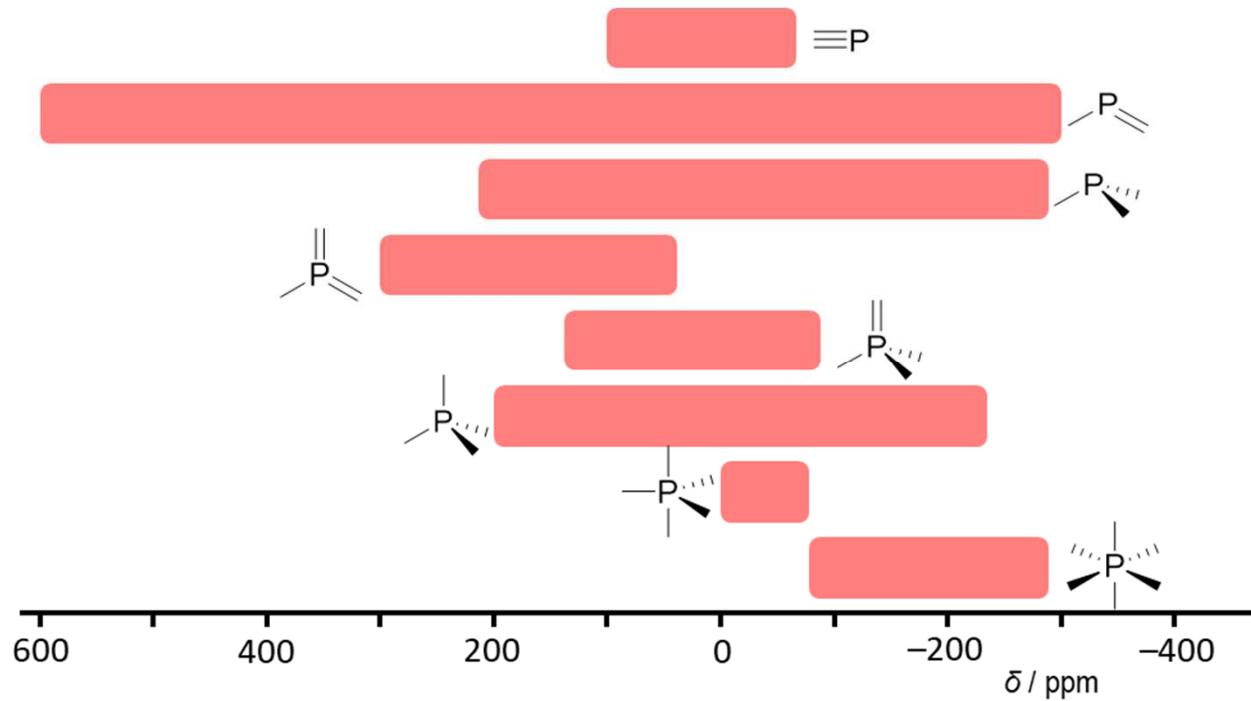


$\text{CF}_3\text{CH}_2\text{OH}$



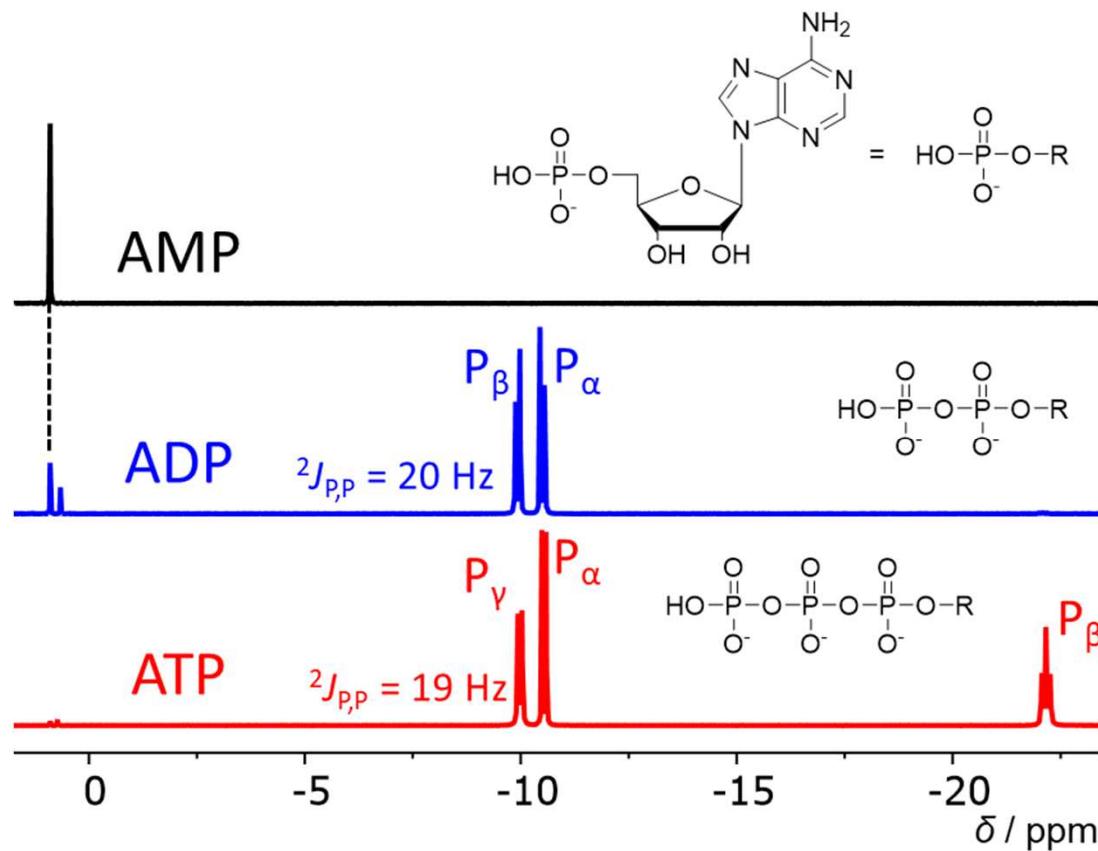
Phosphorus ^{31}P

- 100% natural abundance
- High gyromagnetic ratio (202 MHz on a 500MHz spectrometer)
- High sensitivity
- Large span of chemical shifts

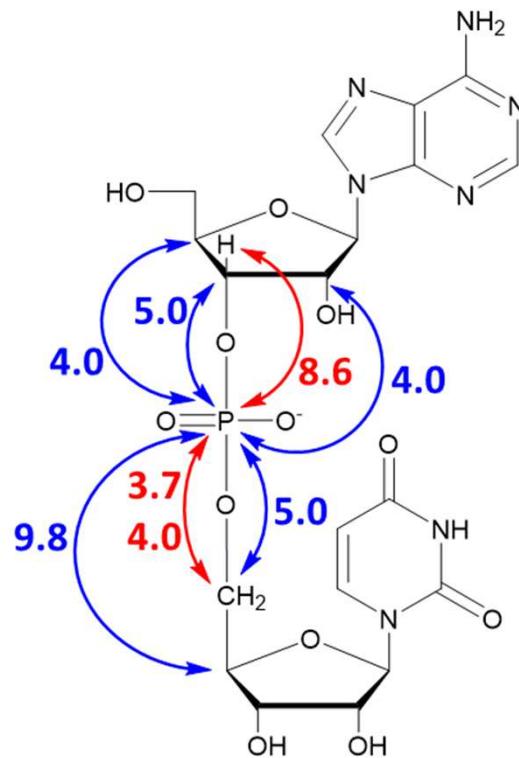


Phosphorus ^{31}P

- $^{31}\text{P}\{^1\text{H}\}$

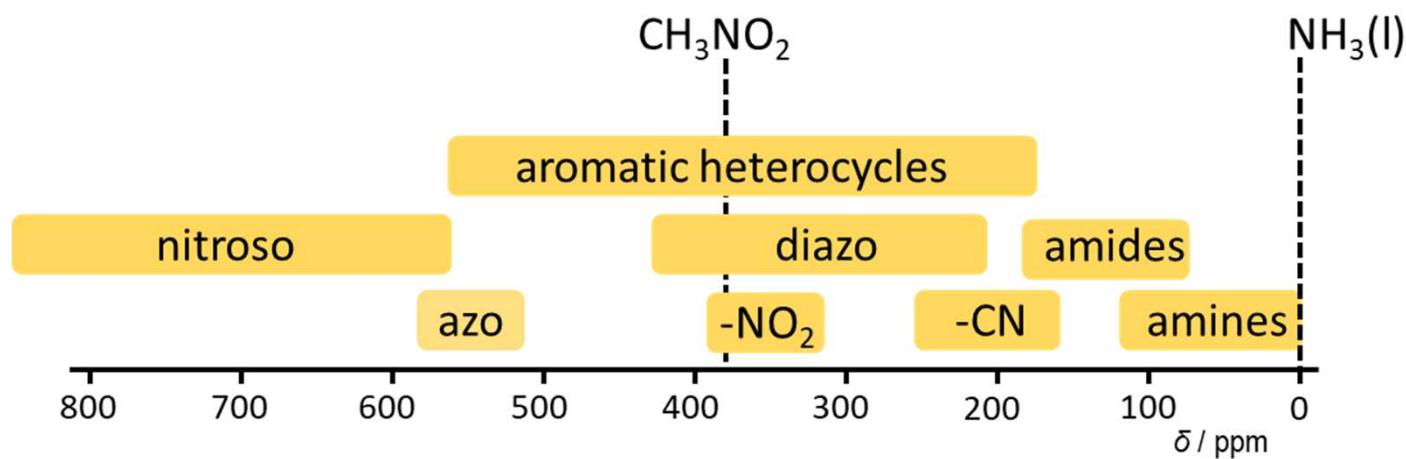


Phosphorus ^{31}P



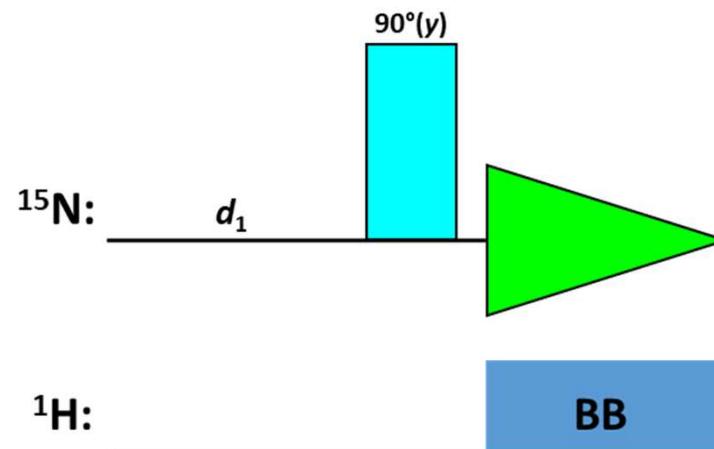
Nitrogen ^{15}N

- 0.37% natural abundance, ^{14}N is quadrupolar
- Low negative gyromagnetic ratio (50 MHz on a 500MHz spectrometer)
- Very low sensitivity
- Large span of chemical shifts, be careful with referencing



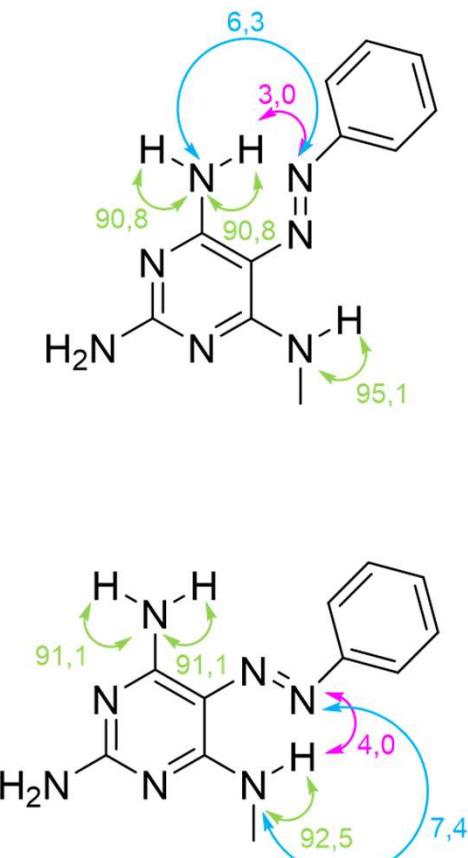
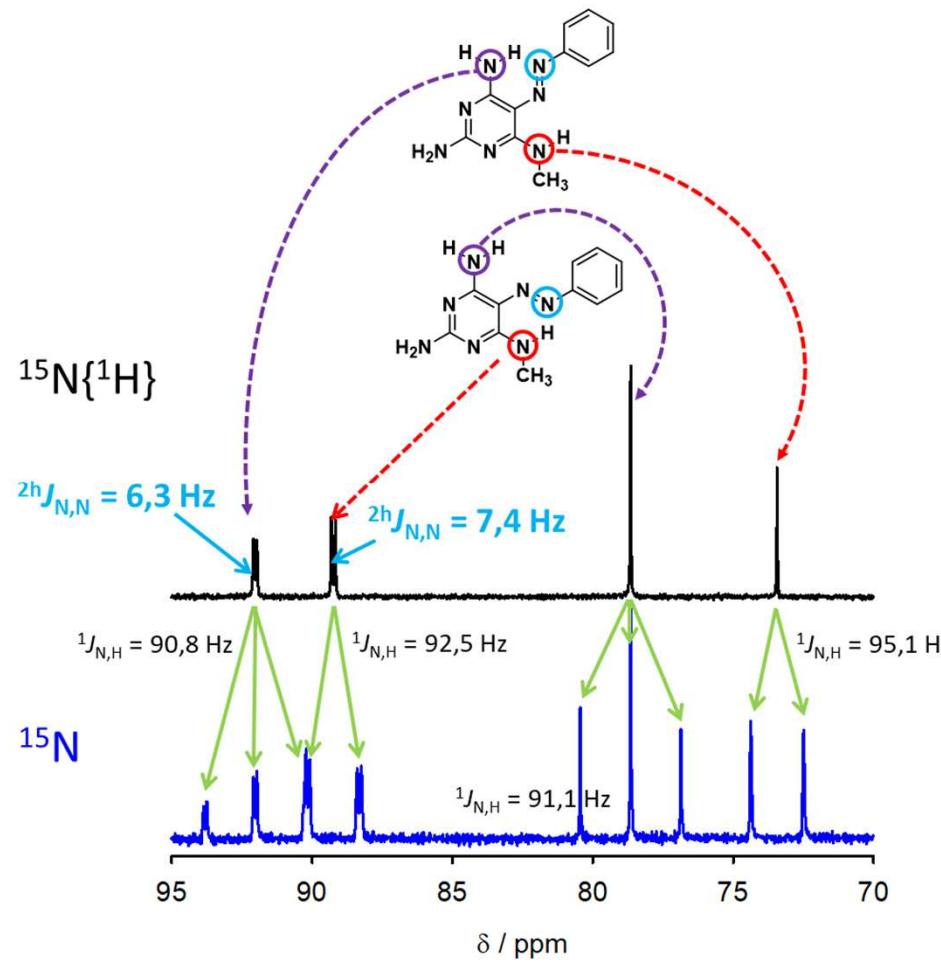
Nitrogen ^{15}N

- 0.37% natural abundance, ^{14}N is quadrupolar
- Low negative gyromagnetic ratio (50 MHz on a 500MHz spectrometer)
- Very low sensitivity, negative NOE
- Large span of chemical shifts, be careful with referencing



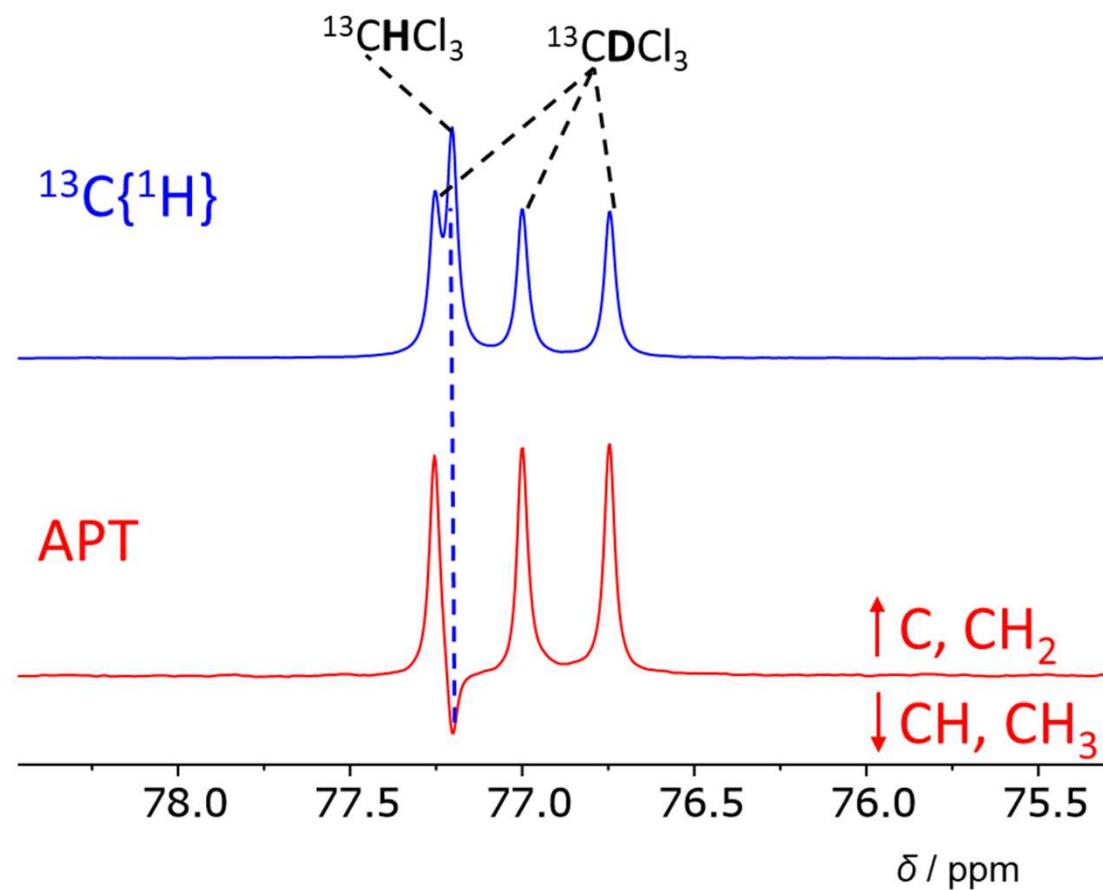
Nitrogen ^{15}N

- Hydrogen bonding, through-hydrogen-bond coupling



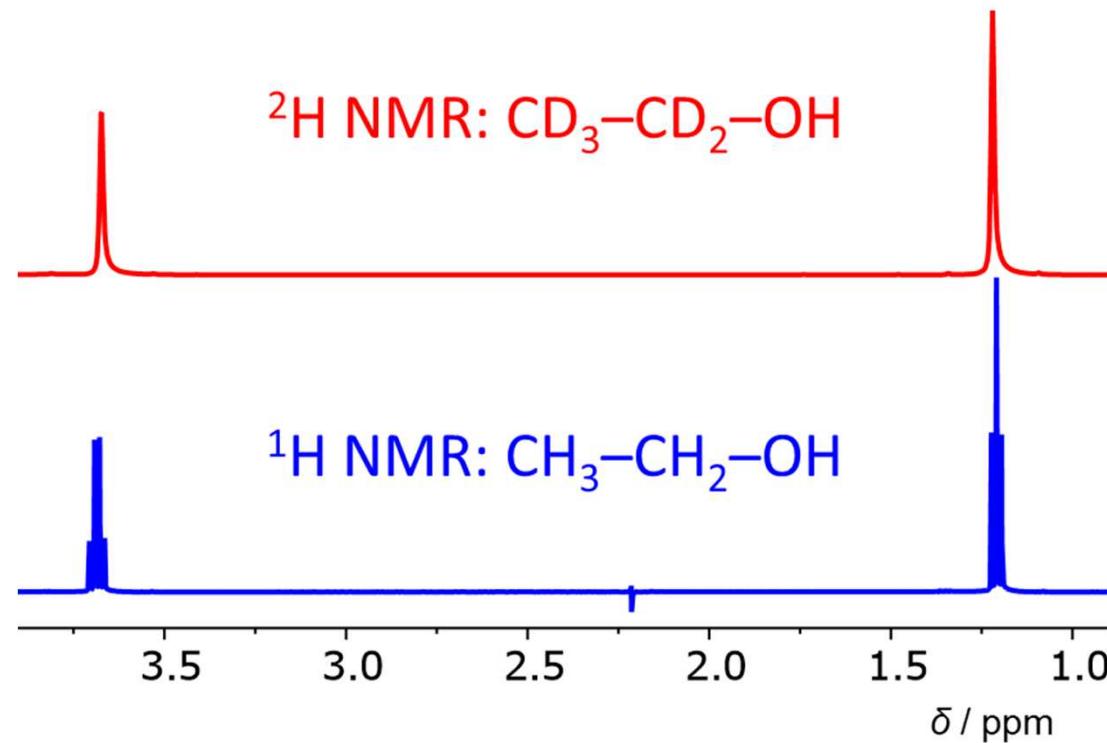
Deuterium ^2H (D)

- Lock, quadrupolar, low sensitivity



Deuterium ^2H (D)

- Lock, quadrupolar, low sensitivity, authenticity of food and beverages



Tritium ^3H (T)

- Radioactive, half-life 12 years
- Highest gyromagnetic ratio (533 MHz on a 500MHz spectrometer)

