Chemistry 3.2
Molecular Spectroscopy

^{13}C Nuclear Magnetic Resonance Spectroscopy (^{13}C NMR)

NMR

- Large magnet aligns all the nuclei along the magnetic field
- The nuclei are then exposed to a series of radiowave pulses
- As the nuclei relax back to its ground state, a radiowave is emitted
- The intensity of the emission is measured against the standard

Carbon Environments

- In ^{13}C NMR, it identifies how many C environment the molecules has
- The number of carbon environments in a molecule depends on the carbon bonding arrangement
  - If two carbon atoms have the same atom connectivity they will only give one peak

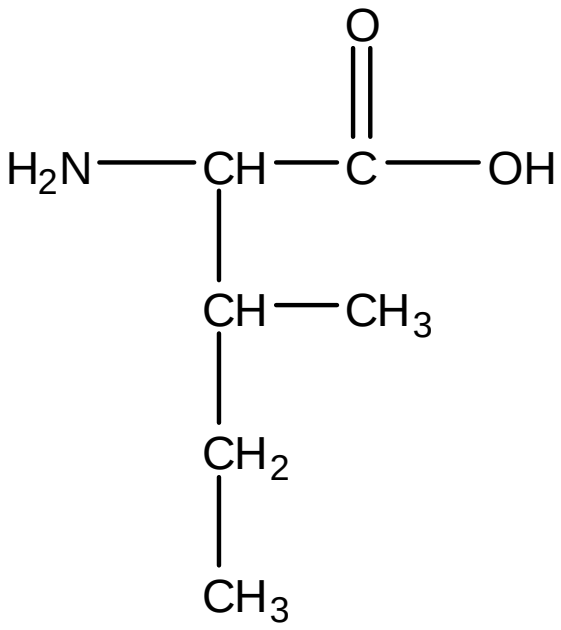
Example

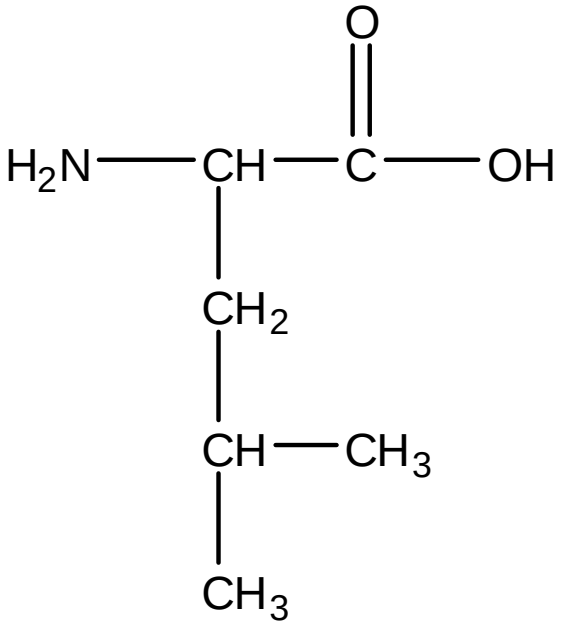
Two amino acids Isoleucine and Leucine

Isoleucine has 6 carbon environments

Leucine has 5 carbon environments

Which one is isoleucine and which one is leucine???





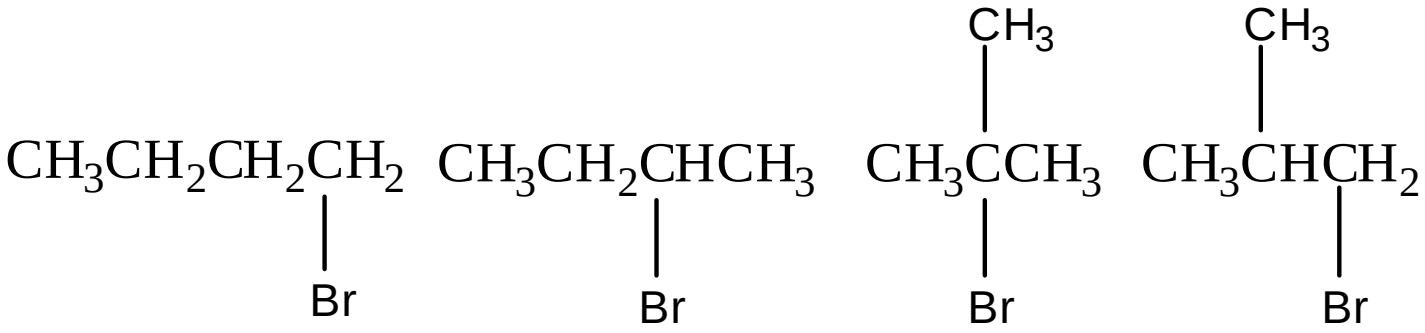
Chemical shift

- Similar to IR, each functional group gives out a particular signal.
- In NMR, the more electropositive carbon, the higher the chemical shift
- A table for chemical shift will be provided in the test

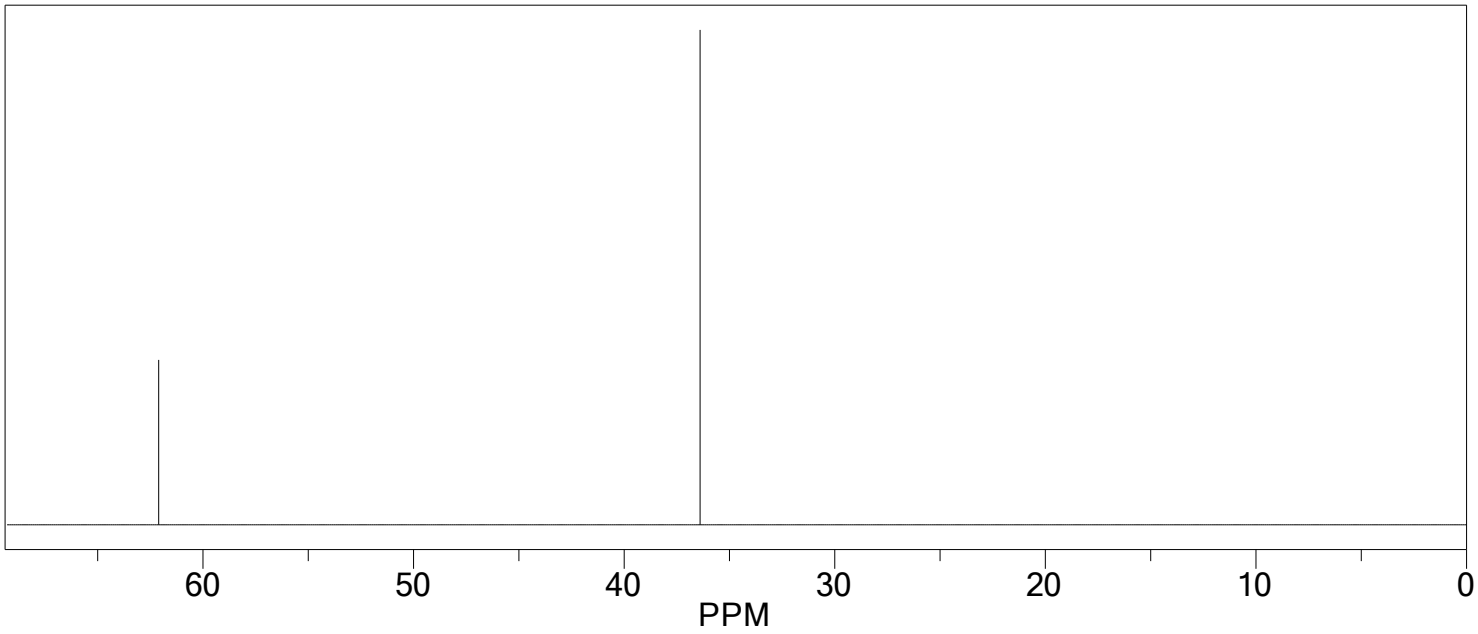
^{13}C NMR Chemical shifts

Carbon environment	chemical shift (ppm)
C=O (in ketones)	205 - 220
C=O (in aldehydes)	190 - 200
C=O (in acids and esters)	170 - 185
C in aromatic rings	125 - 150
C=C (in alkenes)	115 - 140
RCH_2OH	50 - 65
RCH_2Cl	40 - 45
RCH_2NH_2	37 - 45
R_3CH	25 - 35
CH_3CO-	20 - 30
R_2CH_2	16 - 25
RCH_3	10 - 15

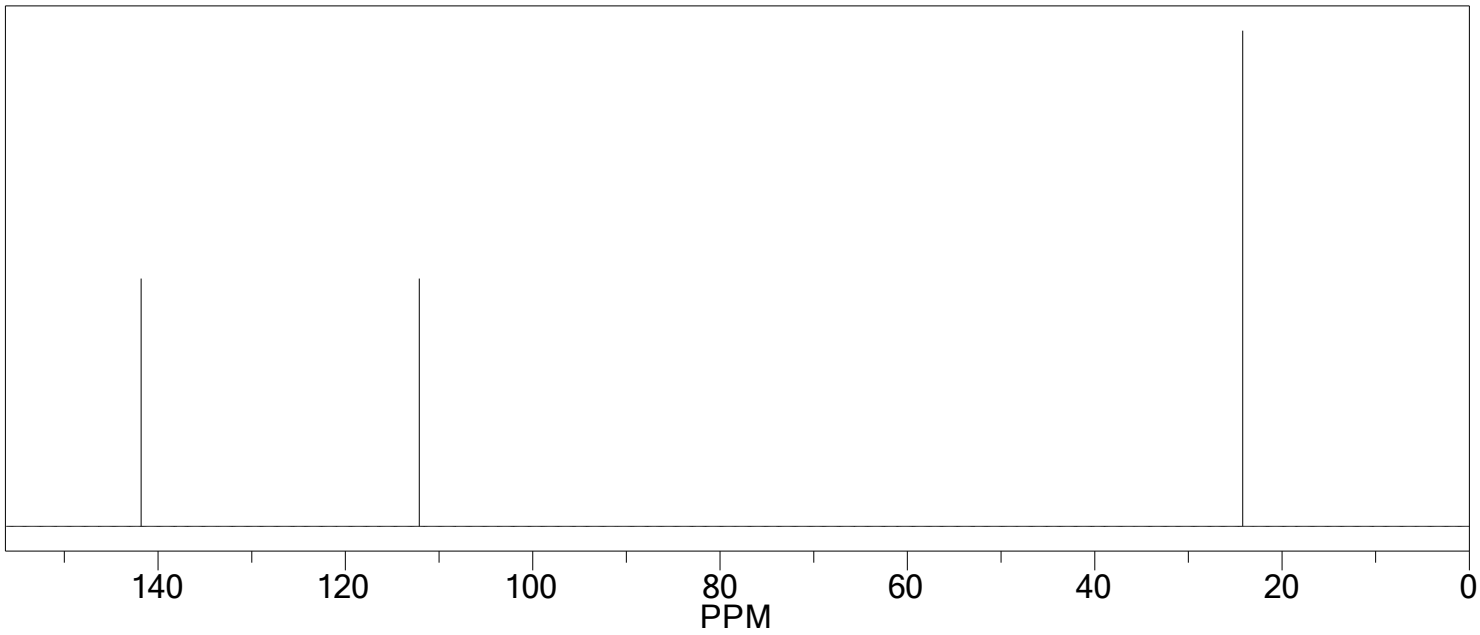
Example



- Determine the number of different chemical environments for the carbon atoms in each of these isomers
- What feature would you expect from a MS spectra of these isomers?



Which isomer in the previous slide corresponds to this spectra?
Circle the carbon responsible for the peak observed in 62.1 ppm



The isomer was exposed to KOH in an unknown condition. The product gives a spectra above.

- What is the condition of the KOH?
- Justify your answers in terms of chemical shift