Spectroscopy Reference Sheet

Unsaturated Number

$$UN = \frac{(2C + 2) - (H + N) - X}{2}$$

C = Carbon H = Hydrogen

N = Nitrogen X = Halides

Common Unsaturated Numbers:

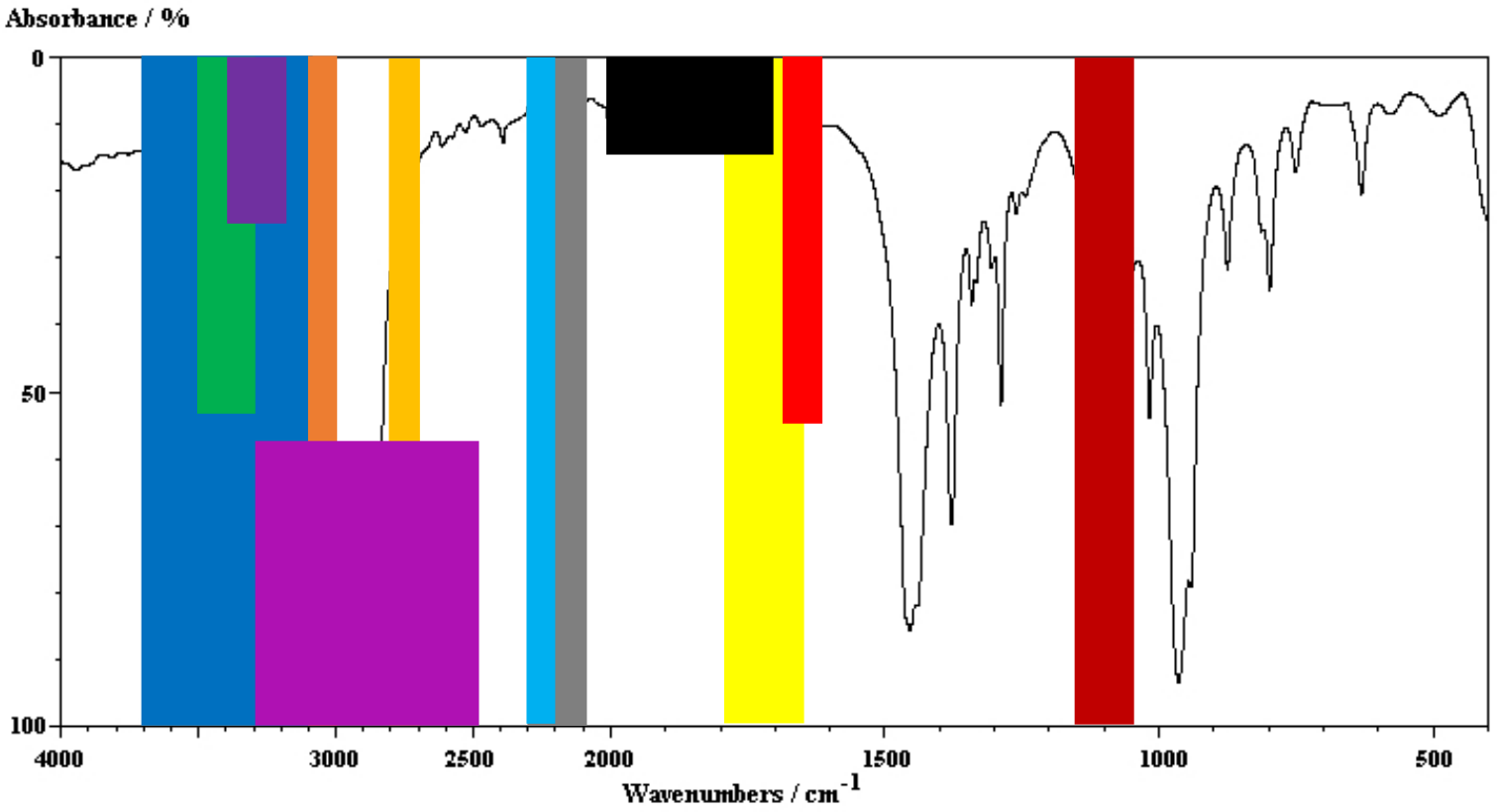
- UN = 0 – NO π Bonds Present
- UN = 1 – Double Bond OR Ring
- UN = 4 – Benzene Ring (3 Double Bond + Ring)
  - Check ^{1}H NMR or IR for confirmation.
- UN = 5 – Benzene Ring + Double Bond
  - Must confirm with ^{1}H NMR or IR

Uncommon Unsaturated Numbers:

ALL UN numbers below must confirm through IR and NMR Spectroscopy

- UN = 2 – Triple Bond, 2 Double Bonds, 2 Rings
  - Potential Combination: Double Bond & Ring
- UN = 3 – Combination: Triple bond, Rings, Double bonds
- UN = 6 – Benzene Ring + Combination
  - Potential Combination: See UN = 2

IR Spectroscopy



- Dark Red – Ether Group (1050-1150 cm^{-1})
- Light Red – Double Bond (1620-1680 cm^{-1})
- Dark Orange – Terminal Alkene (3000-3100 cm^{-1})
- Light Orange – Aldehyde Group (2700-2800 cm^{-1}, 2 Peaks)
- Yellow – Carbonyl Group (1750-1850 cm^{-1})
- Green – Amine Group (3300-3500 cm^{-1})
  - 1° Amine – 2 Peaks
  - 2° Amine – 1 Peaks
  - 3° Amine – 0 Peaks
- Light Blue – Nitrile Group (2200-2300 cm^{-1})
- Dark Blue – Alcohol Group (3100-3700 cm^{-1}, broad)
- Light Violet – Carboxylic Alcohol Group (2500-3300 cm^{-1}, broad)
- Dark Violet – Terminal Alkyne (3200-3400 cm^{-1})
- Gray – Triple Bond (2100-2200 cm^{-1})
- Black – Benzene Ring – Outdated (Multiple Peaks, 1700-2000 cm^{-1})

Possible IR Combinations:

- **Carbonyl + Alcohol = Carboxylic Acid**
- **Carbonyl + Amine = Amide**
- **Carbonyl + Ether = Ester**

^{1}H NMR Spectroscopy

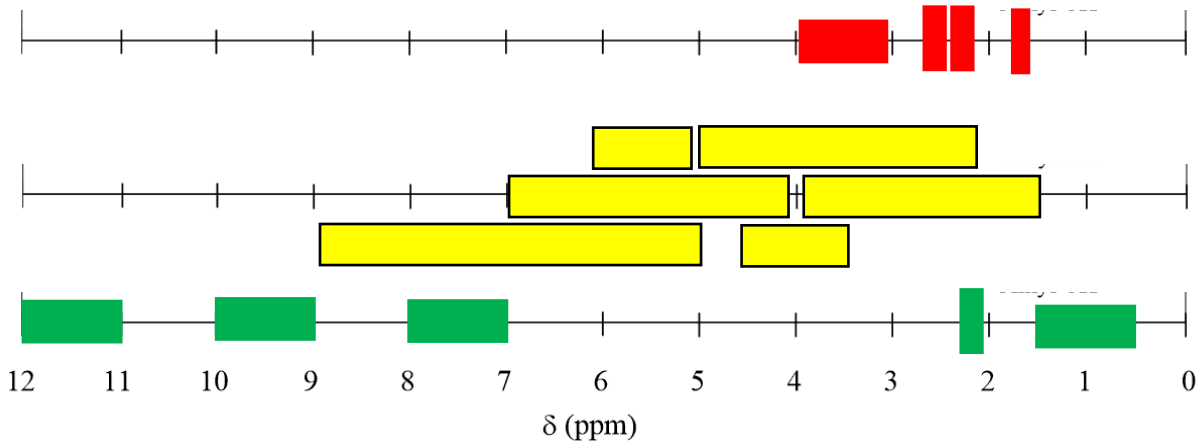
Type of Proton	Approximate δ	Type of Proton	Approximate δ
alkane (—CH_3) methyl	0.9	C=C—CH_3 allylic	1.7
alkane (—CH_2—) methylene	1.3	Ph—H aromatic	7.2
alkane (—CH—) methine	1.4	Ph—CH_3 benzylic	2.3
—C(=O)—CH_3 methyl ketone	2.1	R—C(=O)—H aldehyde	9–10
—C≡C—H acetylenic	2.5	R—C(=O)—OH acid	10–12
R—CH_2—X (X = halogen, O)	3–4	R—OH alcohol	variable, about 2–5
C=C vinyl H	5–6	Ar—OH phenol	variable, about 4–7
		R—NH_2 amine	variable, about 1.5–4

Additional Proton NMR Ranges:

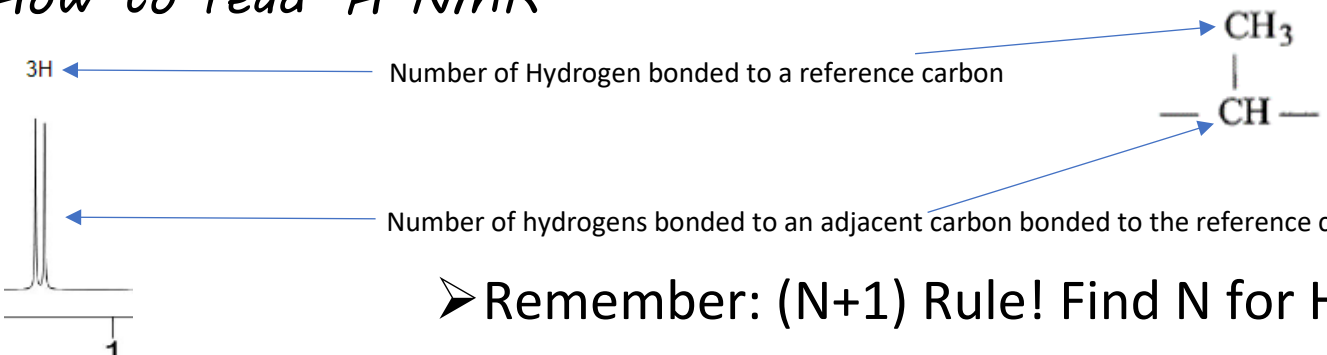
R-O-R-H ether – 3.4-4.5 δ

N-H amide – 5-9 δ

- Green: Must expected to identify!
- Yellow: Must identify based on other peaks
- Red: Extraneous ppm peak indicators



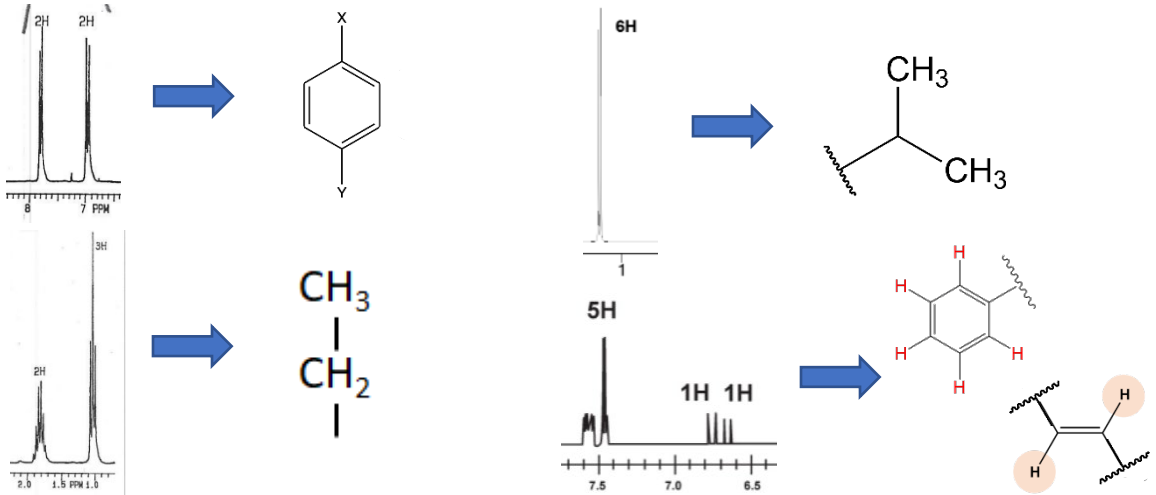
How to read ^{1}H NMR



➢ Remember: (N+1) Rule! Find N for Hydrogen.

Common ^{1}H NMR Peaks

CAUTION: 6H,5H, and double bonds can have varied peaks (watch your ppm!!)



Identifying Compound

ASK YOURSELF:

- Does a certain bond cause a downfield or upfield?
- Did you identify all atoms given?
- Is there peaks where I can combine what the peaks mean?
- Is there any bonds symmetrical for this compound?