Overheads: - Outline

Recap Friday: NMR – what to look for in spectrum (put into table)

1) Number of different H's = # of peaks

2) Chemical Shift (δ):
   - electronegative groups pull ←
   - aromatic H's ~ 7-8; C=C-H ~ 5-6
   - aldehyde ~ 9-10; RCO_2H ~ 10-12

3) Integration: gives relative # of H's in each peak (will be given to you!)

4) Coupling: peaks are split by "n" next-door neighbours into "n+1" peaks
   - singlet (s) = no neighbours, doublet (d) = 1 neighbour;
   - triplet (t) = 2; quartet (q) = 3; quintet, sextet, septet etc

O-H and N-H can exchange with each other (and with D_2O → disappear!))

Problem 1: C_4H_8O U = # rings + double bonds

$$= \frac{(2C + 2 - X + N) - H}{2} \quad (X = \#\text{halogens; } N = \#N)$$

$$= \frac{(2 \times 4 + 2) - 8}{2} = 1 \text{ double bond}$$

IR: 1718 ⇨ C=O

NMR:

δ (ppm)	mult	J	#H	
2.3	q (n=3)	7 Hz	2H	* n = 2 & n = 3 coupled to each other
2.0	s	/	3H	
0.9	t (n=2)	7 Hz	3H	

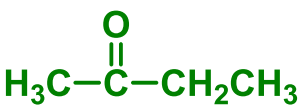
same J if coupled will be given if needed

integrations will be given

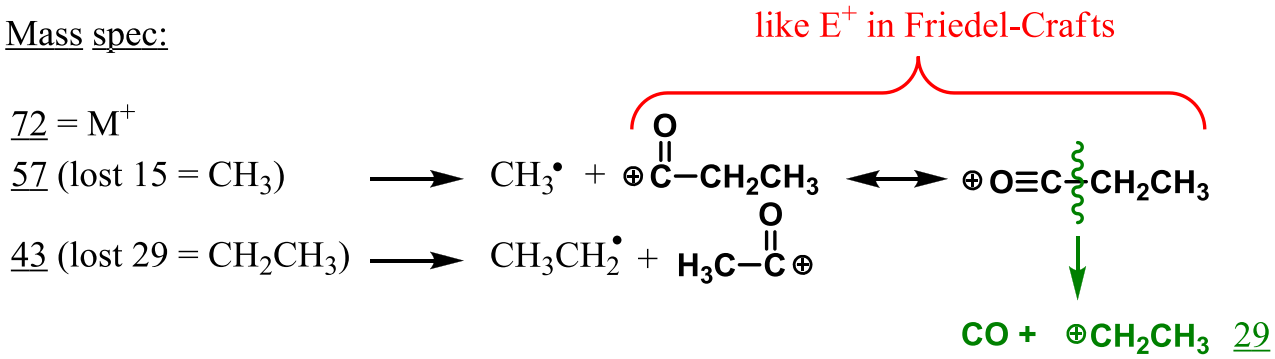
What do we have?

- q / t $-CH_2-CH_3$
- s (3H) $-CH_3$
- IR: C=O

All atoms accounted for!



Mass spec:



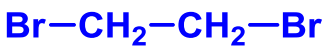
Problem 2: (a) $C_2H_4Br_2$ & (b) $C_2H_4Cl_2$

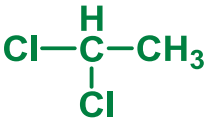
NMR:	δ	mult	#H
	3.7	s	4H

δ	mult	J	#H
5.9	q (n=3)	7 Hz	1 H
2.1	d (n=1)	7 Hz	3H

- All H's same ∴ symmetrical

q / d ∴ -CH-CH_3





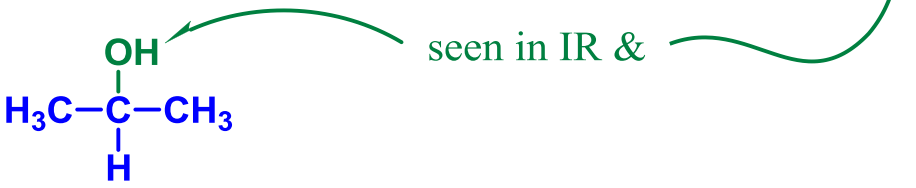
Problem 3: C_3H_8O (no rings or double bonds!)

IR: 3354 – broad ⇨ OH

NMR:	δ	mult	#H (given)
	4.0	septet (n=6)*	1 H
	1.8	s	1H ⇦ exchanges with D_2O ∴ OH!
	1.2	d (n=1)	6H

* note that outer peaks in septet are tiny!

- 4.0 / 1.2 CH coupled to 6H (=2 x CH_3!)



MS: M^+ = 60 (very small – typical for alcohols)