*CHEM 242 – Lecture 23 10/03/2014*

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 ():

- electronegative groups pull 🡨

- aromatic H’s ~ 7-8; C=C-H ~ 5-6

- aldehyde ~ 9-10; RCO2H ~ 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 D2O → disappear!))

Problem 1: C4H8O U = # rings + double bonds

= (2C + 2 – X + N) – H (X = # halogens; N = #N)

2

= (2 x 4 + 2) – 8 = 1 double bond

2

IR: 1718 C=O

NMR: ppm) mult J #H

2.3 q (n=3) 7 Hz 2H \* n = 2 & n = 3

2.0 s / 3H coupled to each other

0.9 t (n=2) 7 Hz 3H

same J if coupled integrations will be given

will be given if needed

What do we have? - q / t -CH2-CH3



- s (3H) -CH3

- IR: C=O

All atoms accounted for!



Problem 2: (a) C2H4Br2 & (b) C2H4Cl2

NMR:  mult #H  mult J #H

3.7 s 4H 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-CH3



Problem 3: C3H8O (no rings or double bonds!)

IR: 3354 – broad OH

NMR:  mult #H (given)

4.0 septet (n=6)\* 1 H

1.8 s 1H exchanges with D2O 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 CH3!)

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



45 (loss of 15 = CH3)