(16) **Today**

Chap 13: Nuclear Magnetic Resonance Spectroscopy

Next Class (17)

Chap 12: Infrared Spectroscopy

Spring Break Begins at 4:30

(18) **Second Class from Today**

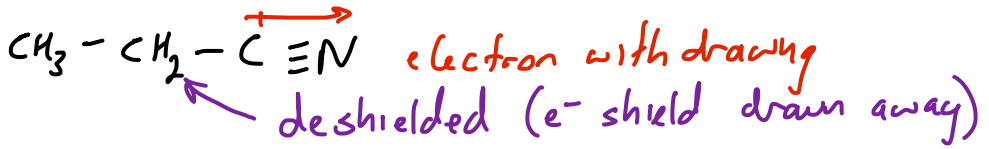
Chap 20 and 21

Third Class from Today (19)

Chap 20 and 21

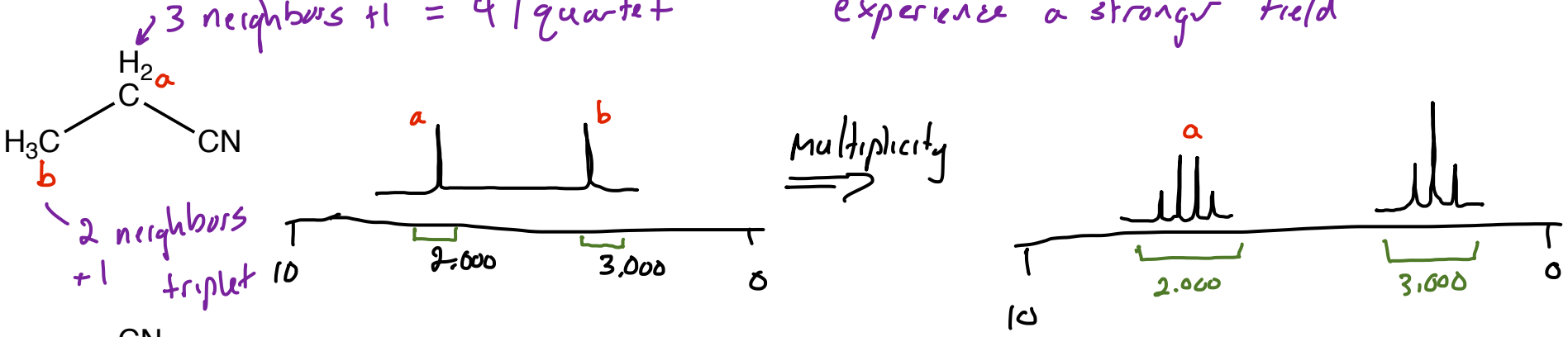
Please rework Test 1 and hand in on March 19.

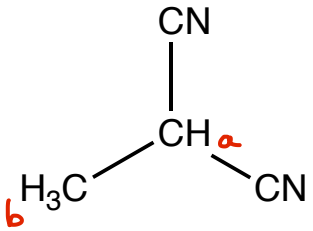
Multiplicity: n + 1 rule



For H to H coupling, the pattern of lines in a peak is n + 1, where n is the number of magnetically equivalent H atoms 3 bonds away from and magnetically inequivalent to the H atoms causing the resonance peak.

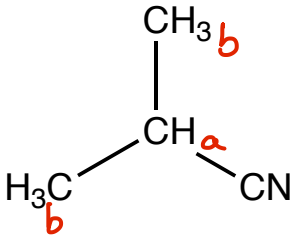
higher resonance frequency because they experience a stronger field





H_a will be a .... quartet (3+1=4)

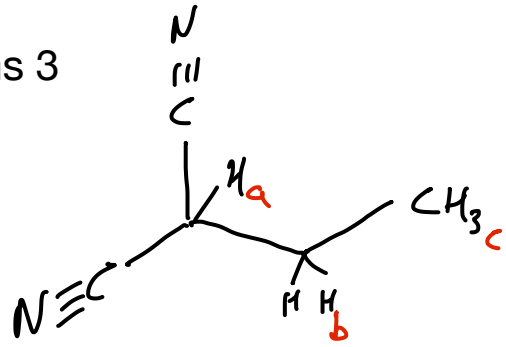
H_b will be a ... doublet (1+1=2)



H_b ... area 6 ... doublet

H_a .... area 1 .... 6 magnetically equivalent neighbors 6+1=7 septet .... but sometimes the ones at the edges are hidden in the baseline

Multiplicity: more than one set of magnetically inequivalent H atoms 3 bonds away

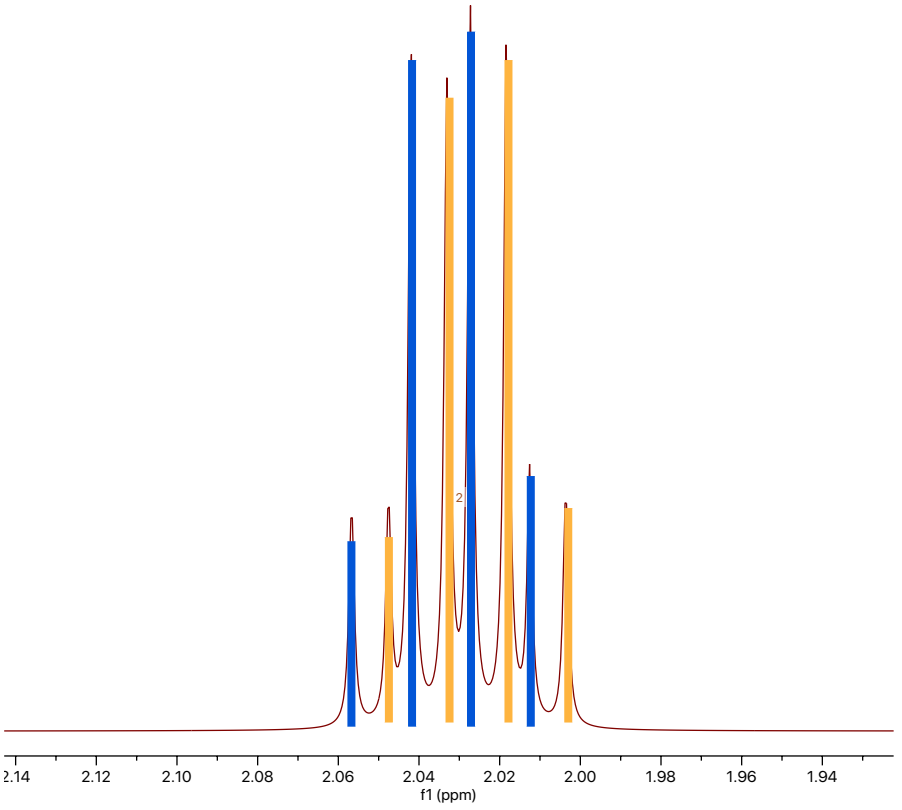


H_b has two magnetically inequivalent sets of neighbors

H_b is split into a doublet by H_a

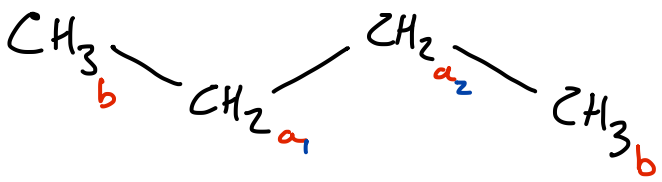
but that doublet is split into a quartet by the 3 H's labled H_c

so H_b is a doublet of quartets



Multiplicity: more than one set of magnetically inequivalent H atoms 3 bonds away

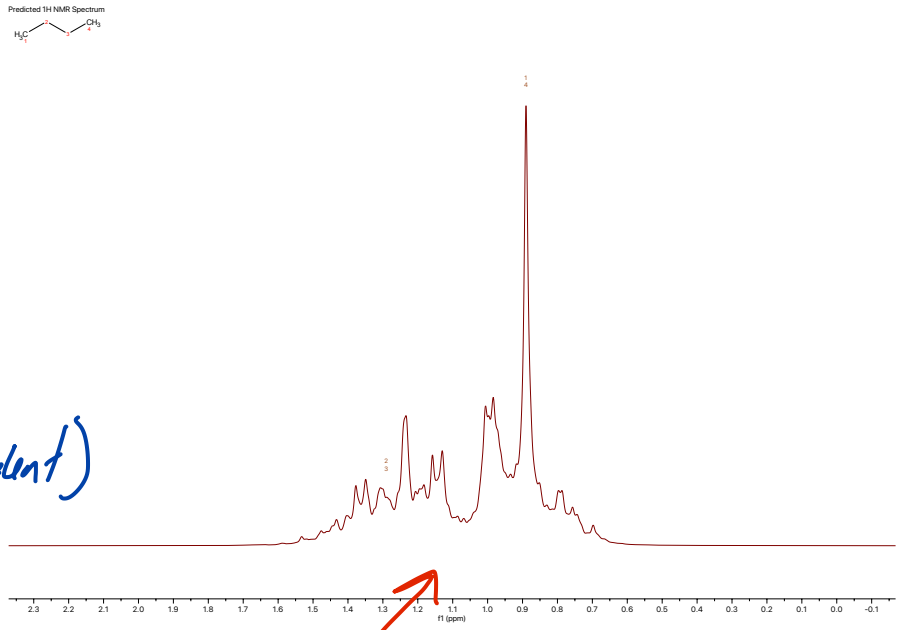
H_b should be a triplet with an area of 6



H_a should be a_1 ....

If a_2 + b are magnetically equivalent ... add them up (3+2) and add 1. (3+2) + 1 = 6

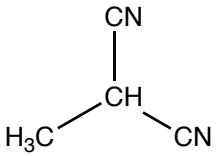
If a_2 + b are magnetically + chemically inequivalent (actually very in equivalent) then (3+1) quartet of (2+1) triplets



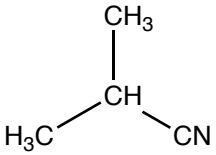
Since these are only a little different .... coupling becomes much more complicated

Multiplicity Summary

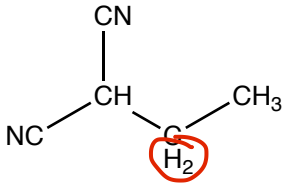
1 set of chemically and magnetically inequivalent neighbors



2 sets of chemically and magnetically inequivalent neighbors that are equivalent to each other



2 sets of chemically and magnetically inequivalent neighbors that are inequivalent to each other

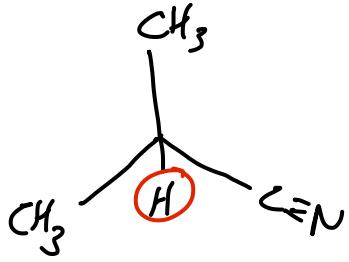


very different

doublet of quartets

not very different

a mess

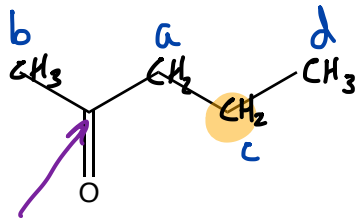


the same septet

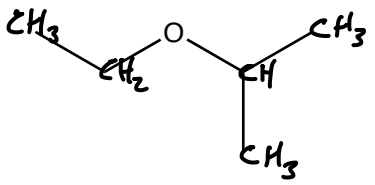
sum all neighbors

Predict Multiplicity

for complicated one's predict "pattern of pattern" an what it would be if it's just 1 pattern



no H here



H_a $(2+1)=3$ triplet, t

H_b $(0+1)=1$ singlet, s

H_c $(2_l+1)=3$ t $(3_r+1)=4$ q; so a tq

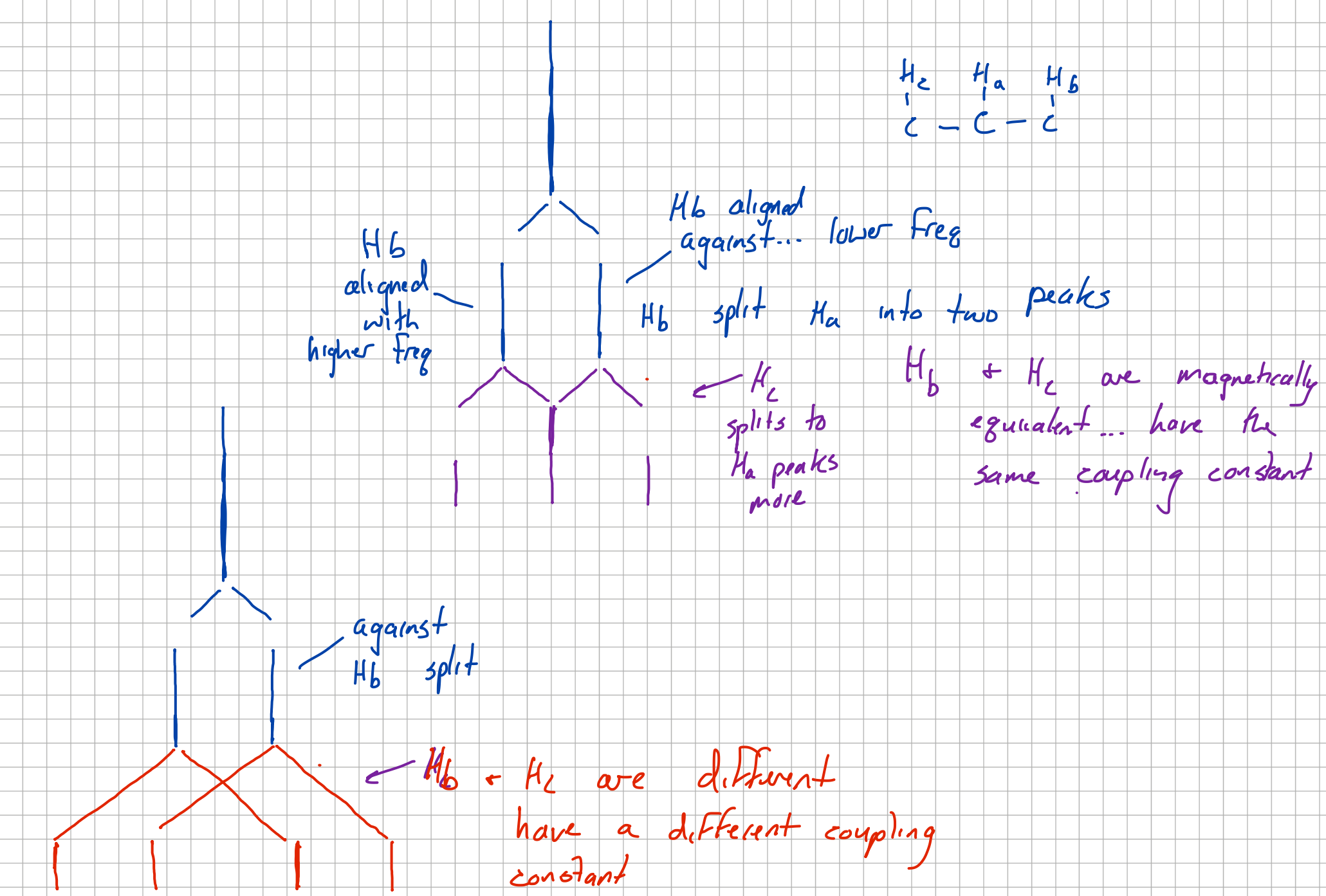
mess

$((2+3)+1)=6$ sextet

} with H's like these consider what all the possibilities are

H_d $(2+1)=3$ triplet, t

4 peaks


H_c H_a H_b
C – C – C
H_b aligned against... lower freq
H_b aligned with higher freq
H_b split H_a into two peaks
H_c splits to H_a peaks more
H_b & H_c are magnetically equivalent... have the same coupling constant
against H_b split
H_b & H_c are different
have a different coupling constant