(15) **Today**

Chap 13: Nuclear Magnetic Resonance Spectroscopy

Next Class (16)

Chap 13: Nuclear Magnetic Resonance Spectroscopy

(17) **Second Class from Today**

Chap 13: Nuclear Magnetic Resonance Spectroscopy

Third Class from Today (18)

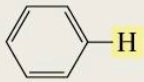
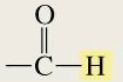
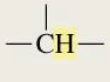
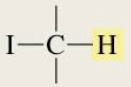
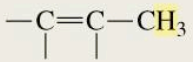
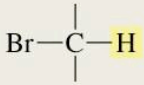
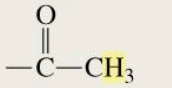
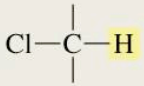
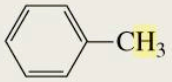
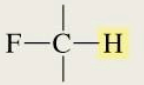
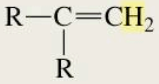
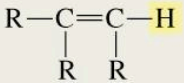
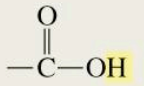
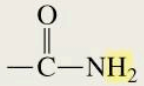
Chap 12: Infrared Spectroscopy

Spring Break Begins at 4:30

Please rework Test 1 and hand in on March 19.

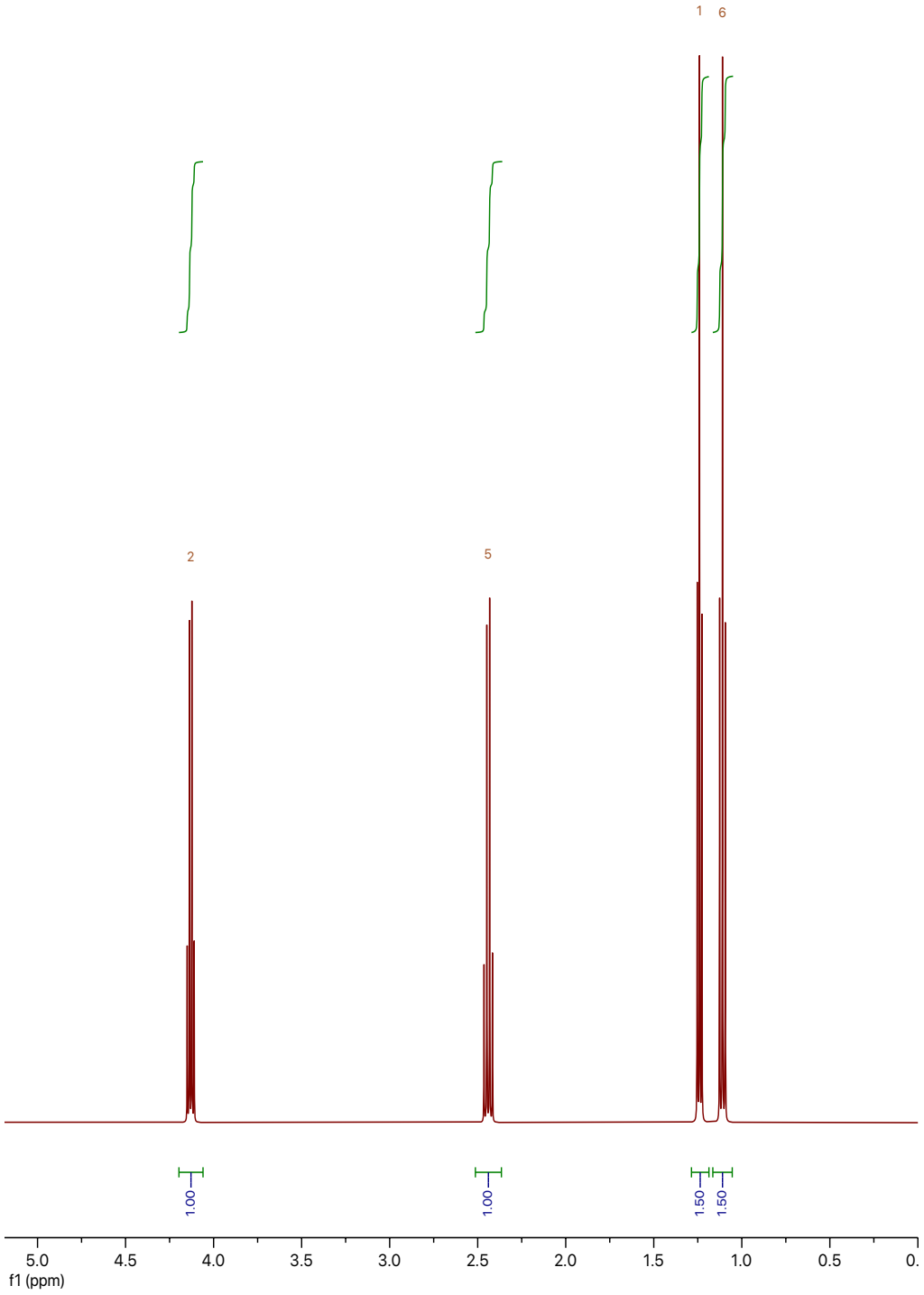
Characteristic Chemical Shifts

Table 14.1 Approximate Values of Chemical Shifts for ^{1}H NMR[a]

Type of proton	Approximate chemical shift (ppm)	Type of proton	Approximate chemical shift (ppm)
$(CH_3)_4Si$	0		6.5–8
$-CH_3$	0.9		
$-CH_2-$	1.3		9.0–10
	1.4		2.5–4
	1.7		
			2.5–4
	2.1		
			3–4
	2.3		
			4–4.5
	2.4		
	3.3	RNH_2	Variable, 1.5–4
	4.7	ROH	Variable, 2–5
		ArOH	Variable, 4–7
	5.3		Variable, 10–12
			Variable, 5–8

[a]The values are approximate because they are affected by neighboring substituents.

What Does the Integration Tell Us?

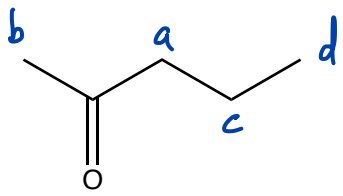


Integration: What ratios will the computer give us if the smaller peak is assigned an area of 1?

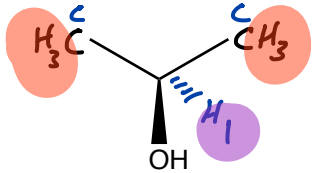
a : b : c : d

2 : 3 : 2 : 3

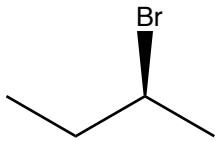
1 : 1.5 : 1 : 1.5 } ratio of area

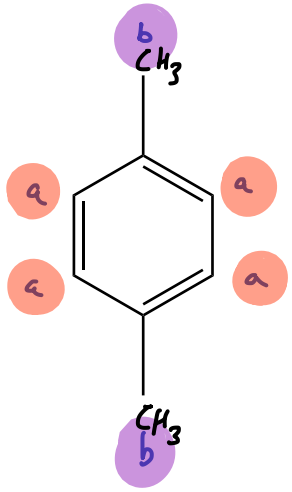


6



1

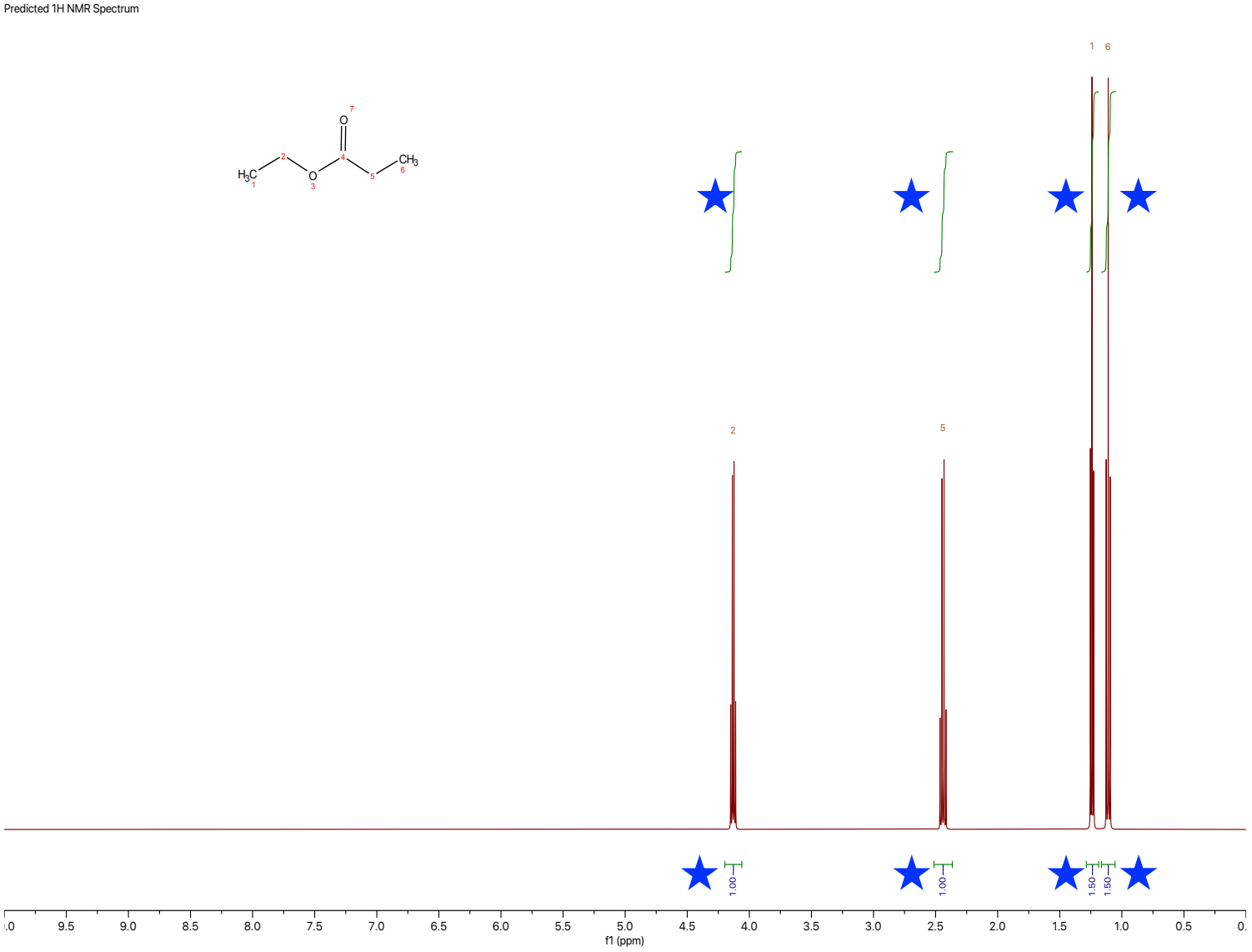




6 1.5

4 1

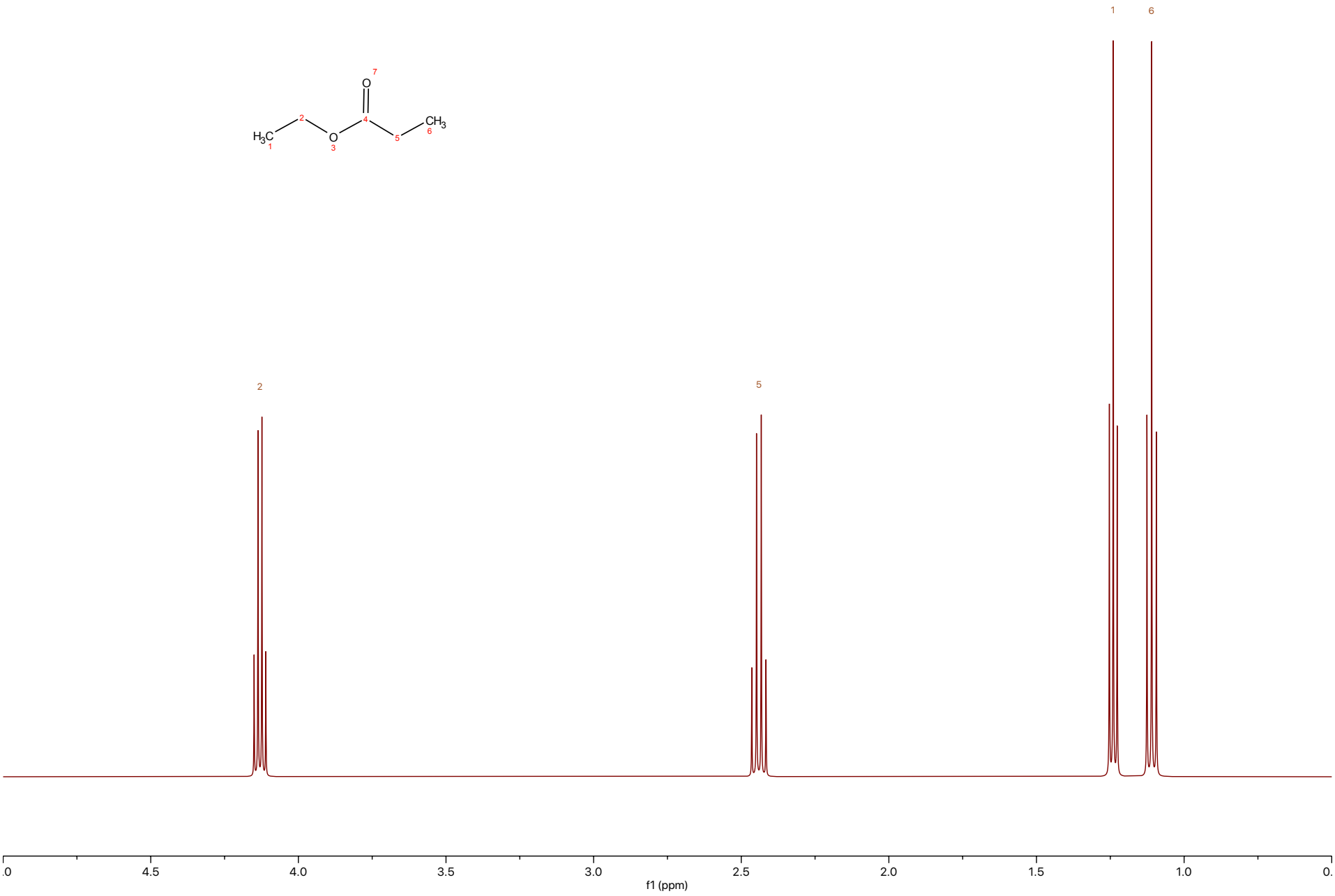
The NMR Spectrum



# of different types of H atoms	Chemical environments of the H atoms	How many of each type of H atom	# of H atom neighbors
number of peaks	position of peaks	★ integration of peaks	

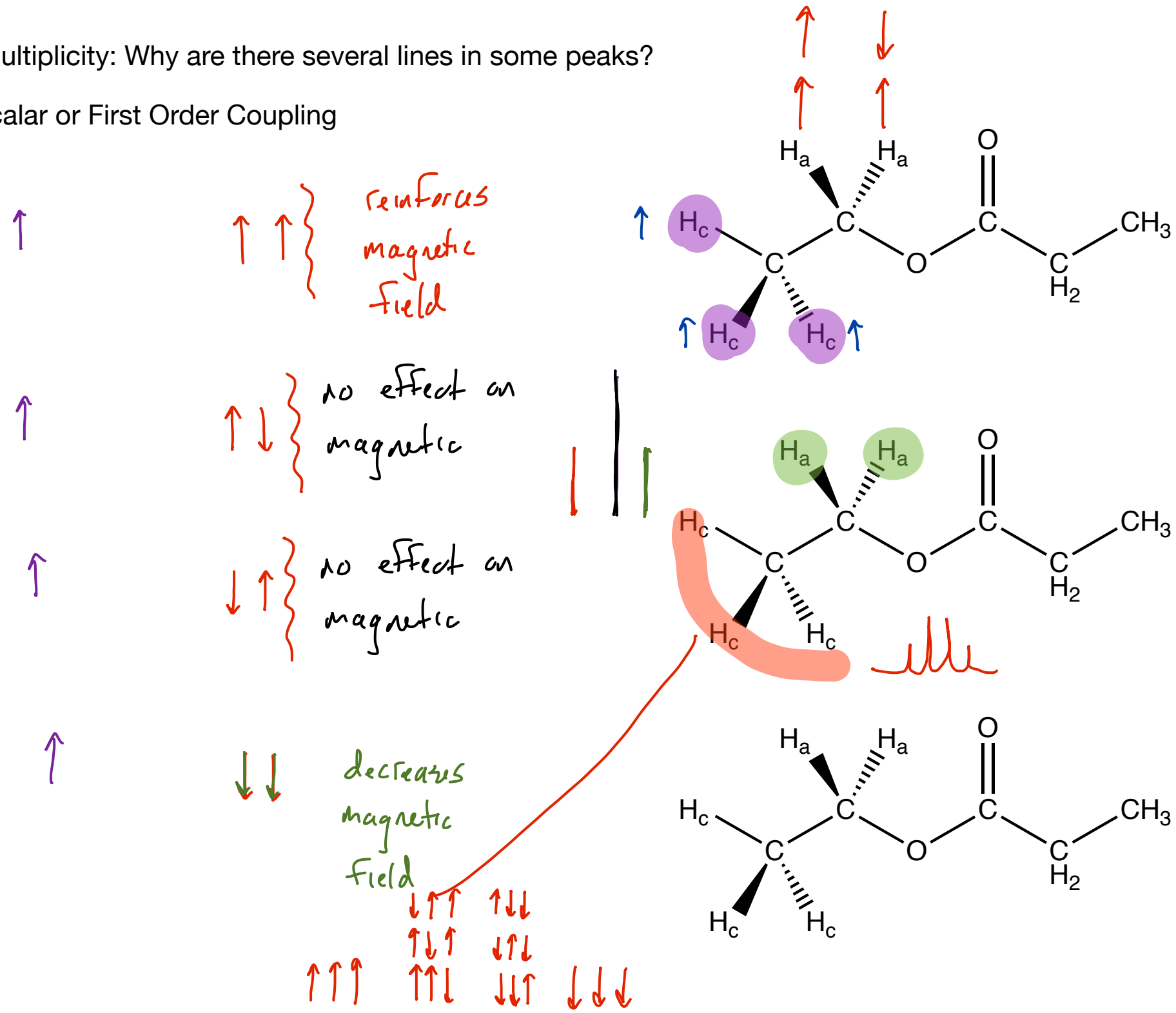
Multiplicity: Why are there several lines in some peaks?

Predicted 1H NMR Spectrum



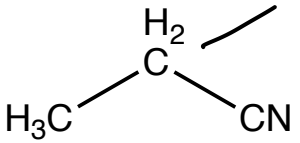
Multiplicity: Why are there several lines in some peaks?

Scalar or First Order Coupling



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.

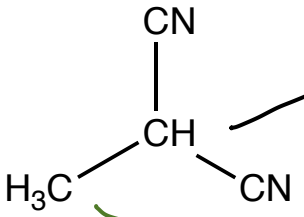


what pattern? the neighboring C to the right has no H's

The neighboring C to the left has 3 H atoms

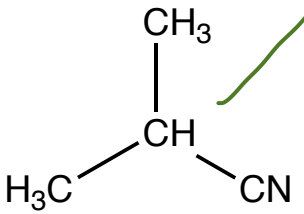
(3+1) = 4 the CH_2 will be a quartet

what pattern? triplet (2 H's as neighbor)



quartet

1 H on neighboring C, so 2 lines... doublet



3 neighbors up top ... 3 neighbors lower left

CH_3's in this molecule are chemically and magnetically equivalent, so add them up septet 6+1 = 7

multiplet