CHEM 222 section 01

LECTURE #12

Thurs., Oct.11, 2007

Lecture topics & readings

Today's class

- NMR spectroscopy (Ch.13)

Before next class

- read sections 13.8-13.12

Next class

- finish NMR (?)

(1)

13.9 Integration of NMR signals ⇒ relative #s of Hs



Note: integration is a crucial part of interpretting NMR data

- UV/Vis and IR peaks are not integrated
- MS peaks are integrated, but yield less-than-crucial information



13.10 Peak shape: splitting of signals follows "N+1" rule

Spin-spin coupling: ¹Hs feel magnetic fields of adjacent ¹Hs

- equivalent Hs not affected by each other (yield same signal ...)
- ¹Hs on adjacent atoms (\leq 3 bonds away) *coupled* to each other
- coupled ¹H's split each other's signal



Back to 13.10... Peak multiplicity follows the "N+1 rule": #peaks in signal = (#coupled Hs) + 1

# Equivalent ¹ Hs causing splitting	Multiplicity of the signal	f Relative peak intensities	Table 13.2
0	singlet	1)
1	doublet	1:1	
2	triplet	1 : <mark>2</mark> : 1	Pagaalia
3	quartet	1 : 3 : <mark>3 : 1</mark>	trianale
4	quintet	1 : 4 : 6 : <mark>4</mark> : 1	
5	sextet	1 : <mark>5 : 10</mark> : 10 : 5 : 1	
6	septet	1 : 6 : <mark>15</mark> : 20 : 15 : 6 : 1	J

Sketch an expected spectrum for diethyl ether:

(5)



13.12 Coupling constants can identify "partners"

Spin-spin coupling: causes equal spacing between peaks in multiplet
to identify coupling partner ⇒ find other multiplet with same spacing

spacing in Hz = coupling constant (J)







Coupling constants can help with stereochemistry too

Summary so far: information provided by ¹H NMR spectra

FEATURE	INFORMATION LEARNED
# of signals	# of different kinds of H atoms in molecule
Chemical shift	Type of H & neighbouring substituents • CH ₃ , CH ₂ , CH • EWGs • allylic, vinylic • aromatic • aldehyde
Integration	Relative # of H of each type
Multiplicity <i>(N+1)</i>	# of equivalent Hs (N) bonded to adjacent Cs
Coupling constants	Identify coupled protons

