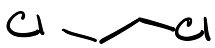
Chemical Equivalents

How many unique chemical environments there are in a molecule

Both for proton & carbon

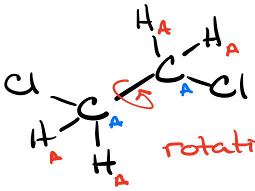
Symmetry

Examples



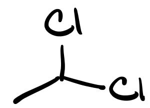
1,2-dichlorethane

=



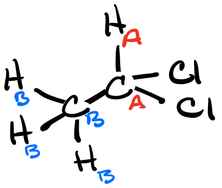
rotation about σ bonds

^{1}H-NMR environments	^{13}C-NMR environments
1	1

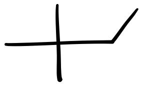


1,1-dichlorethane

=



H environments	C environments
2	2



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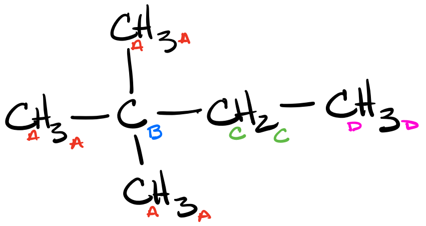
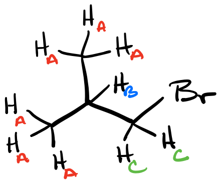


$CH_3-\underset{CH_3}{\overset{CH_3}{C}}-CH_2-CH_3$

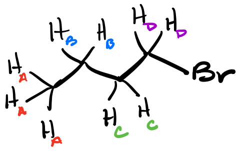
H environments
3

C-environments
4



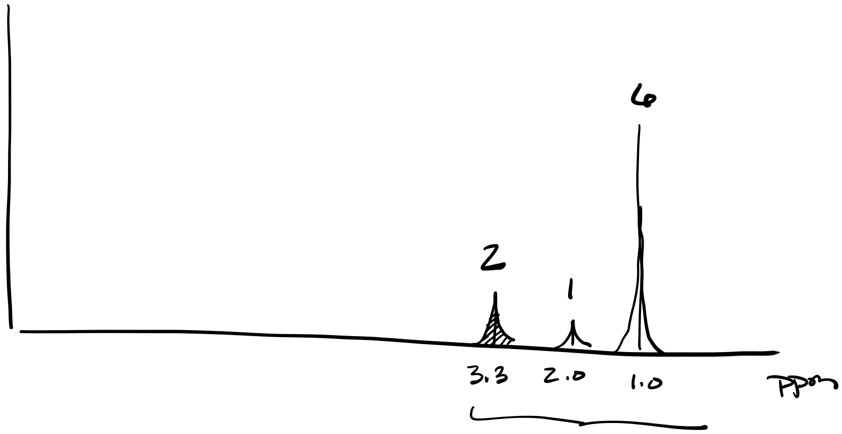
^1H Environments 3

vs



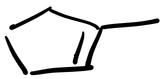
4

^1H-NMR (Simple - Spin decoupled)

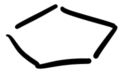


3 environments

A



B

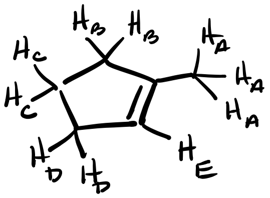


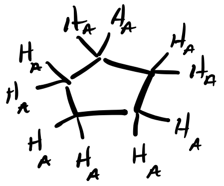
C

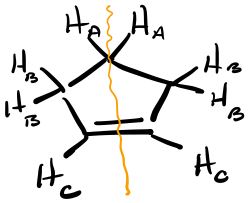
How many

	A	B	C
' H environments	5	1	3
^{13}C environments	6	1	3

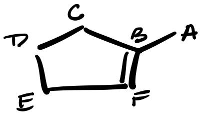
5

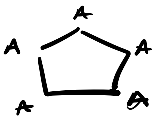


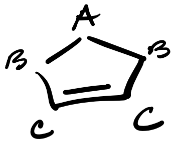


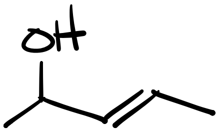


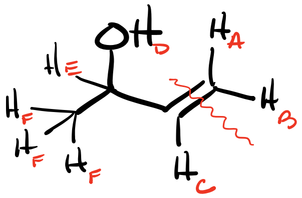
6



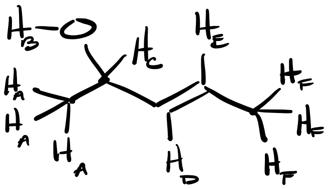


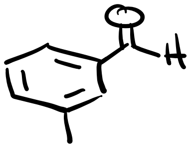


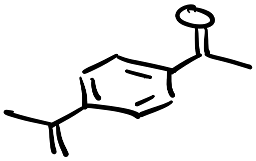




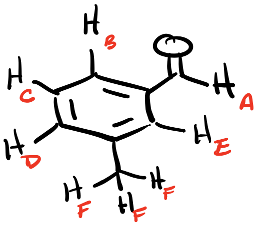
H environments	6	6
C environments	5	4

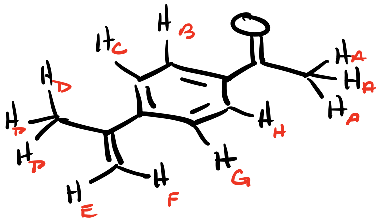


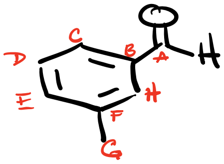


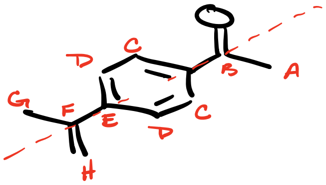


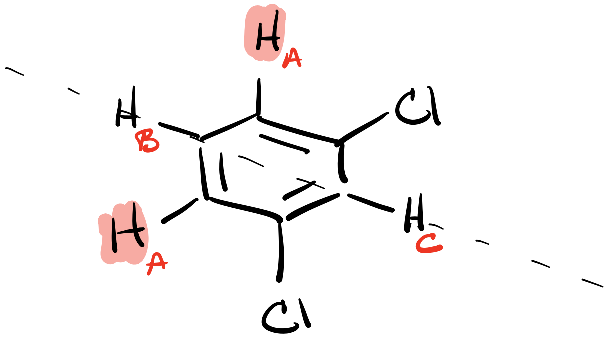
H environments	6	8
C environments	8	8

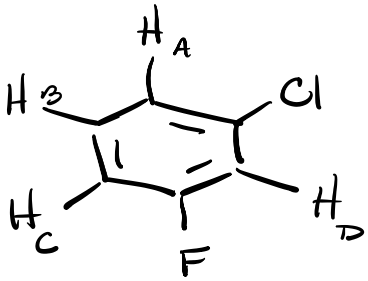


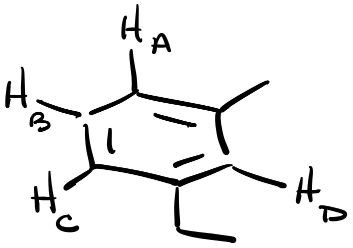


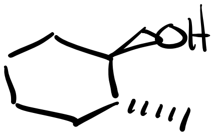




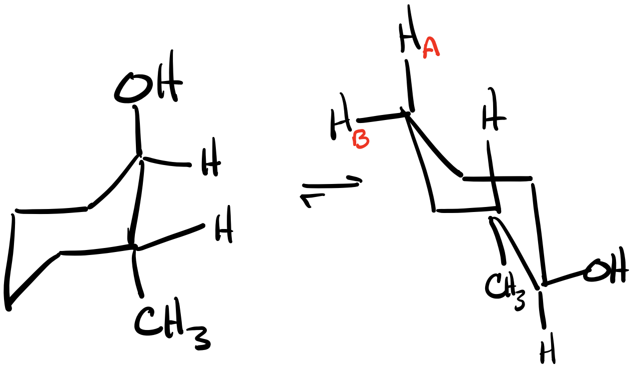




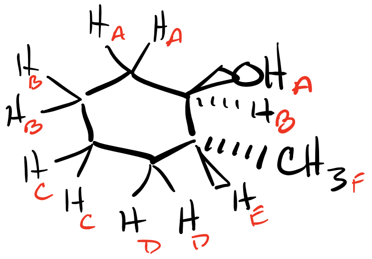


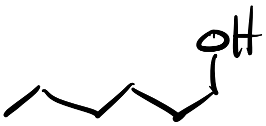


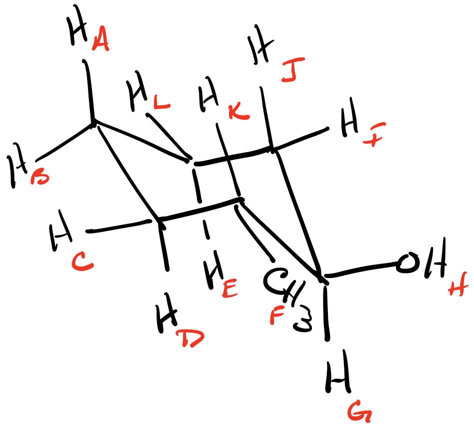
Environments	
^{1}H	8
^{13}C	7



major

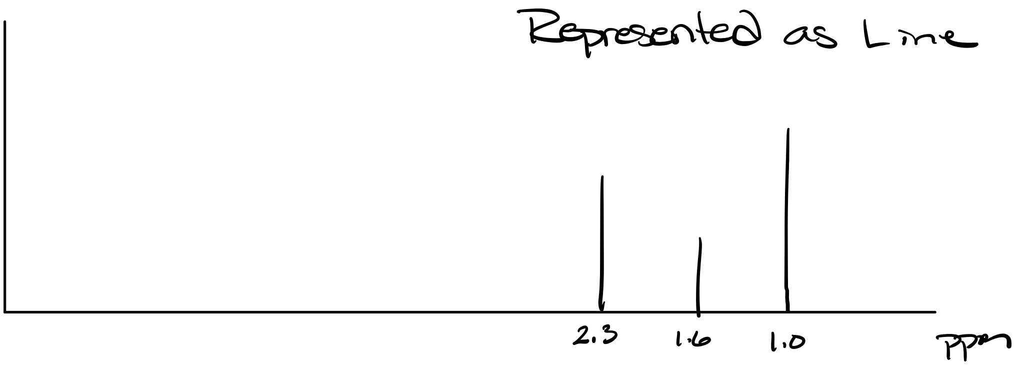


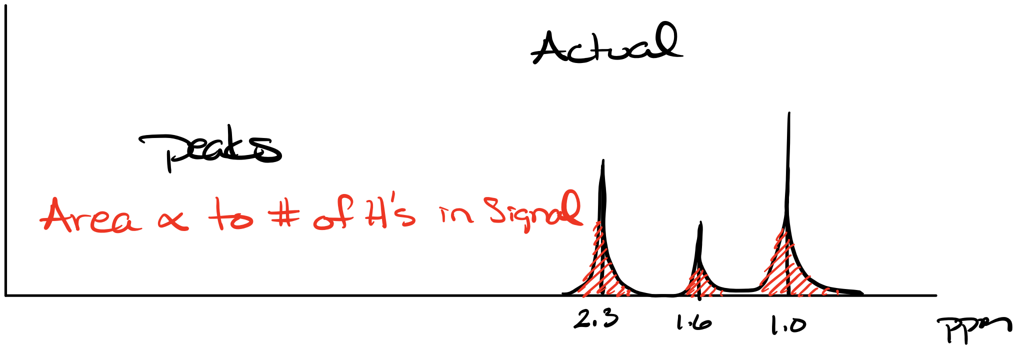




Integration

^1H-NMR


Represented as Line


Actual

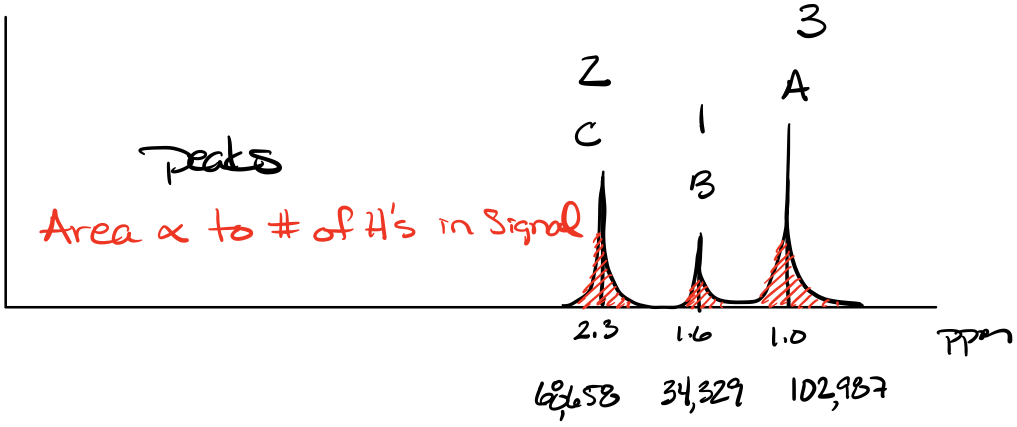
Peaks

Area ∝ to # of H's in Signal

Raw integrations are just that, they are raw areas ppm * Intensity

Raw integrations must be converted into relative Integrations

Actual



Relative Int

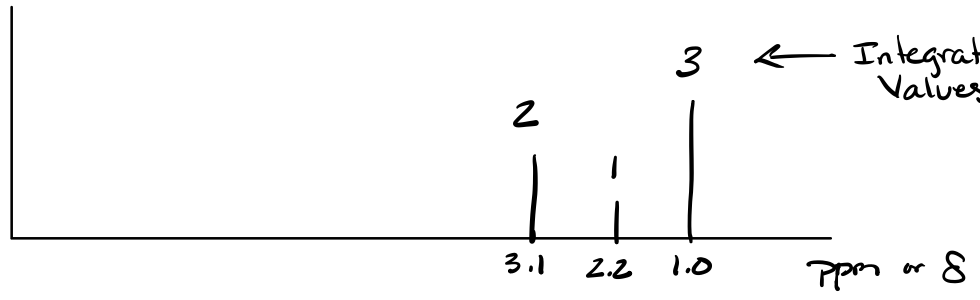
A $\frac{102,987}{34,329} = 3$

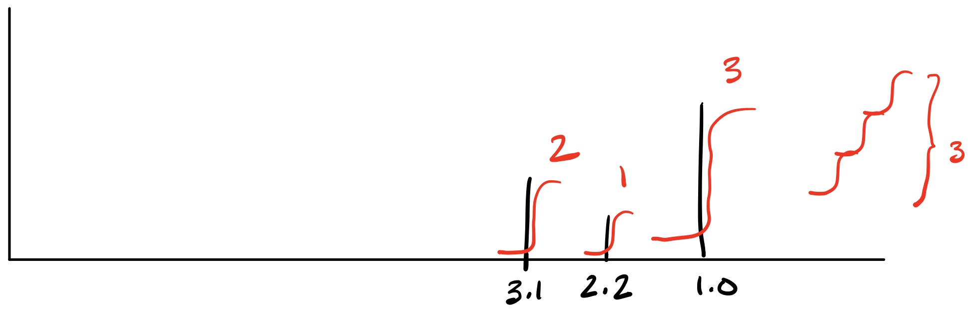
B $\frac{34,329}{34329} = 1$

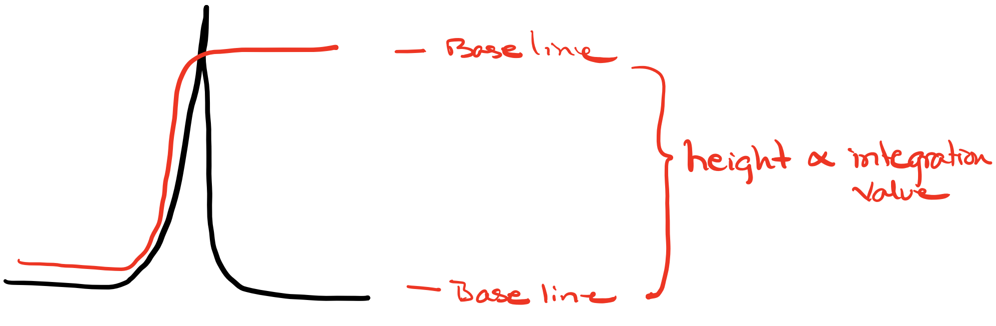
C $\frac{68,658}{34329} = 2$

Ratios & Could be
3 : 1 : 2
6 : 2 : 4
9 : 3 : 6

Ways Integrations are Communicated







Only ^{1}H-NMR can be integrated

^{13}C-NMR <u>can not</u> be integrated

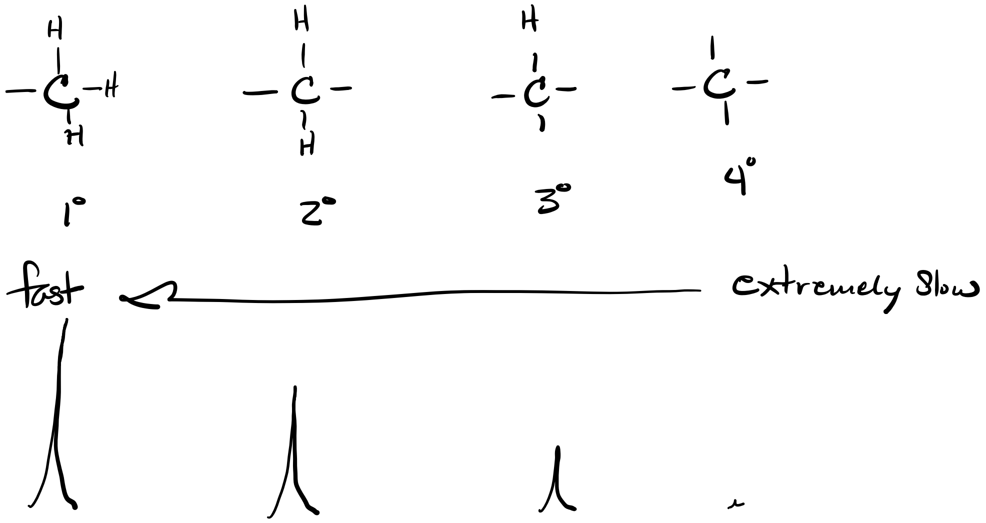
Reason

Protons have fast relaxation times.

They all relax at similar rate

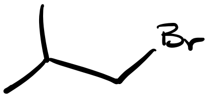
Size of peak ∝ to # H's giving rise to peak

Carbons don't relax at same rate

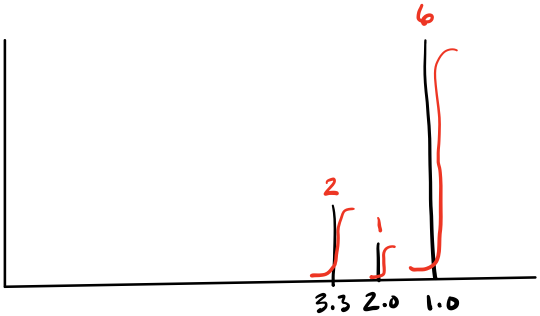


only the fastest carbons relax fully

250 MHz NMR w/ $CDCl_3$ Solvent

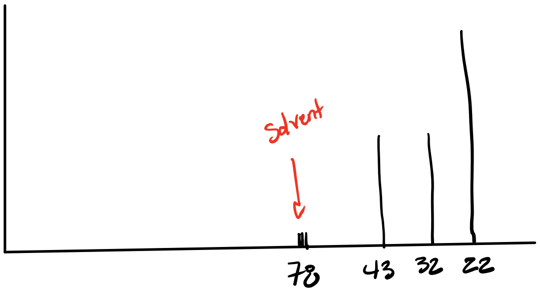


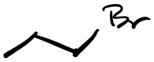
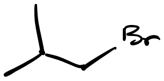
^{1}H-NMR
Environments = 3



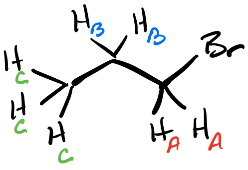
$\boxed{2:1:6}$

^{13}C-NMR
Environments = 3

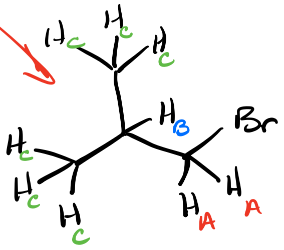


Chemical Environments		
H	3	3
C	3	3

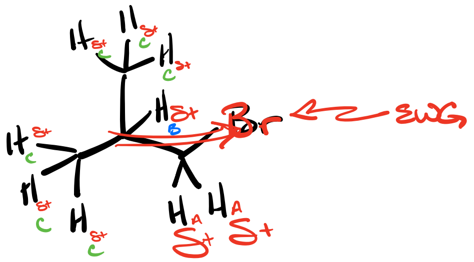
Ratios

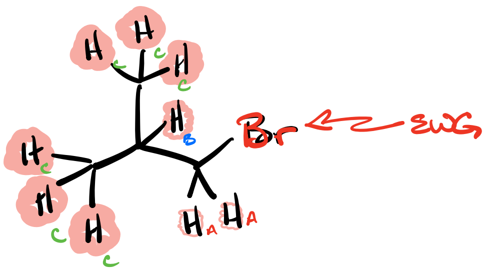


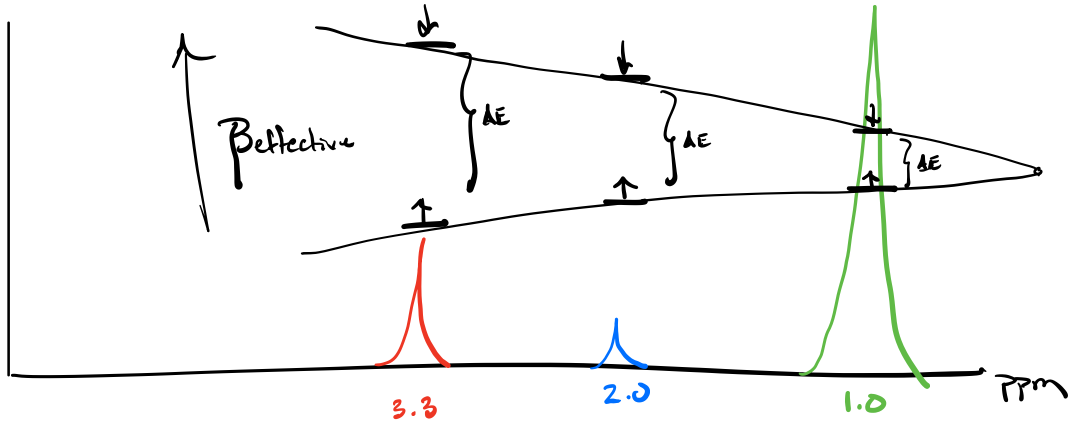
C	B	A
3	2	2



C	B	A
6	1	2







← Downfield
Deshielded

upfield →
Shielded