NMR

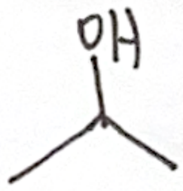
^1H NMR → tells us "type" and "relative Hs" of Hs in molecules

- chemical equivalence
- ratio area under the ~~curve~~ curve
- "Adjacent ^1H Nuclei → splitting
- $e^{\ominus}$ density around a given ^1H nuclei ⇒ chemical shift

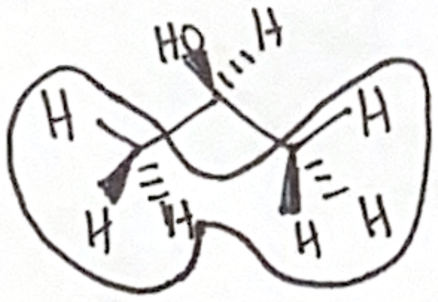
① chemical equivalance:

Equivalent sets of ^1H atoms

↳ <u>same chemical environment</u> ⇒ H atoms are bound to the "same things"



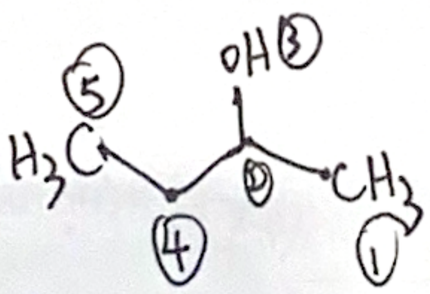
All bonds in this molecule rotate freely. → <u>single bonds</u>, <u>no rings</u>



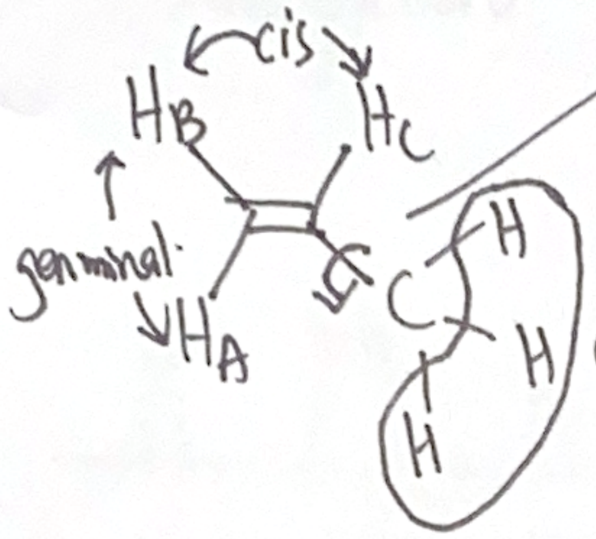
3 sets of chemically equivalent H-atoms.

⇓

3 signals in the NMR



5 signals



→ This bond can rotate freely.

chemically equivalent.

4 sets of H atoms → 4 signals

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what H_B feels ?

cis to Hc

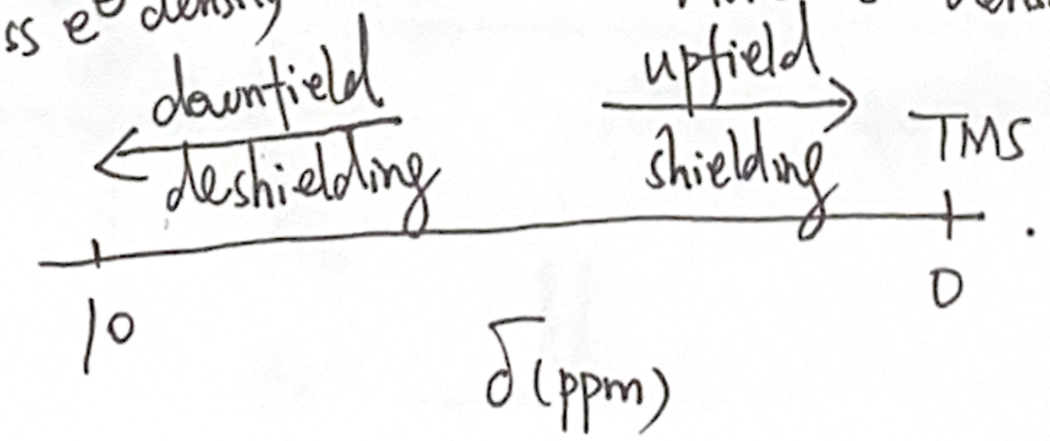
Seminal to ~~Hc~~ H_A

trans to CH_3

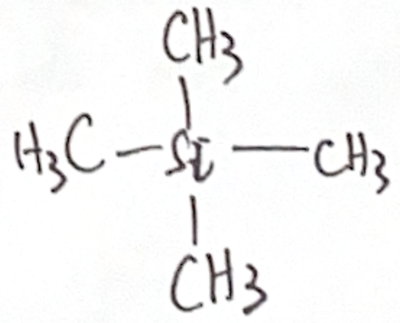
② chemical shift. (ppm)

changes in $e^\ominus$ density around a H atom due to E.N atoms nearby that pull $e^\ominus$ density away

less $e^\ominus$ density → more $e^\ominus$ density



TMS :



define 0 ppm

③ Integration $\int dx \Rightarrow$ area under curve

area: 140 280 140

Ratio: 1 : 2 : 1

1H : 2H : 1H

2H : 4H : 2H

⋮

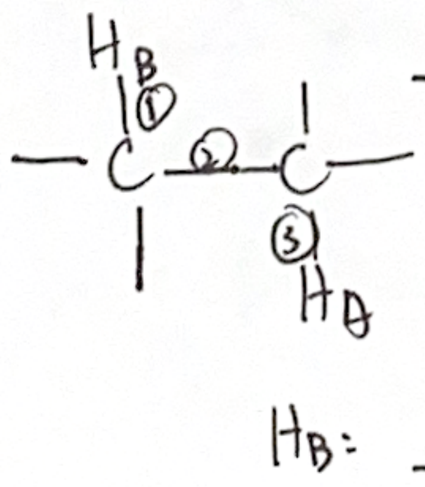
Relative amount of H-atoms that correspond → a signal

↳ ratio of the # of sets of chemically equivalent H-atoms

④ splitting → "adjacent" ^1H nuclei change the net magnetic field felt by a given/different ^1H nucleus

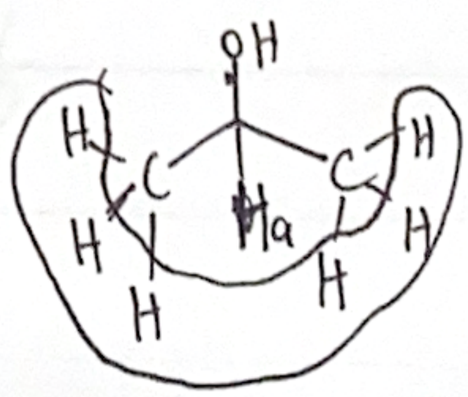
↳ tells us how many "non-equivalent" H-atoms are adjacent

3 bonds or fewer

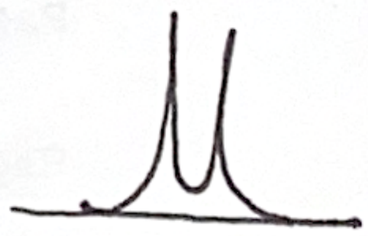


H_B: 

Note: equivalent H-atoms do not split each other



1 signal of 6 Hs, don't split each other

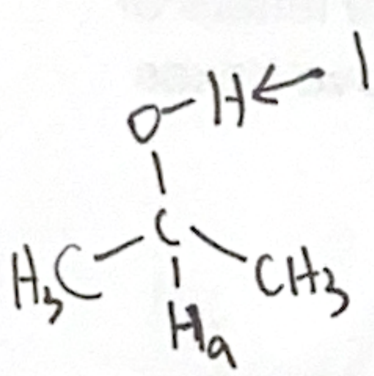


For ^1H on freely spinning C-atoms:

# of peaks in the split signal = n+1

n = # of "adjacent" non-equivalent H-atoms
(that aren't on -OH, $-NH_2$)

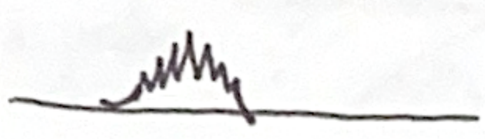
Broad peaks that aren't split, and doesn't split adjacent nuclei

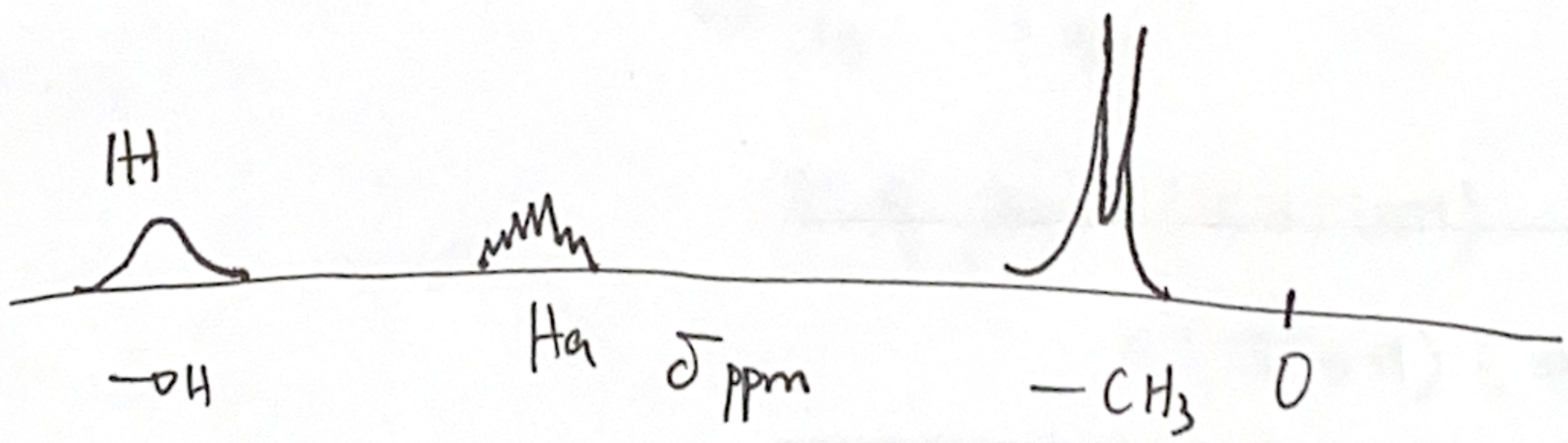


← 1 broad signal, no split

{ 1 H atom
{ 1 signal → integrate to 1H

adjacent Hs: 6 n=6, 7 peaks





1 : 1 : 6

Non-freely rotating C-atoms (Alkenes, small rings)

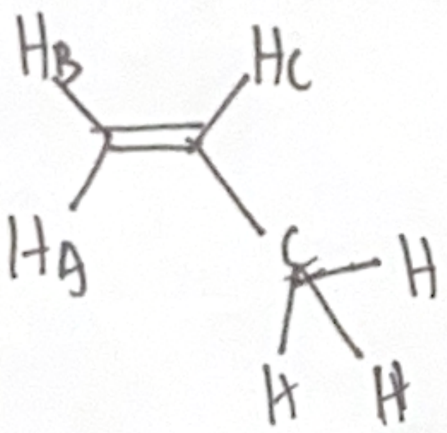
↳ multiplicative splitting.

# of peaks = $(n+1)\cdot(m+1)\cdot(p+1)\ldots\ldots$

where n is the # of <u>one set</u> of chemical ~~shift~~ equivalent H-atoms

m ..... another set of .....

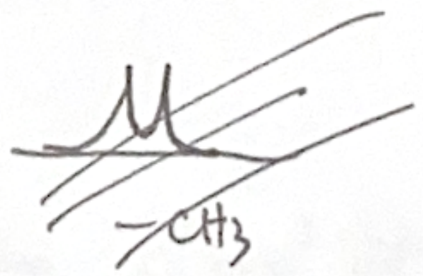
etc.



4 signals:

1) $-CH_3$ 3 # atoms

$n+1 = 1+1 = 2$ peaks



2) H_A 1 H

# of peaks = $(m+1)(n+1)$

$= (\#H_B+1)(\#H_C+1)$

$= (1+1)(1+1) = 4$ peaks

3) H_B 1H

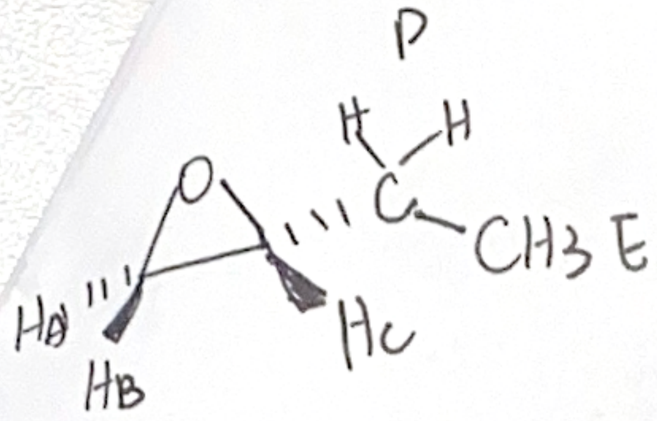
# of peaks = $(\#H_A+1)(\#H_C+1)$

$= 2\times2 = 4$ peaks

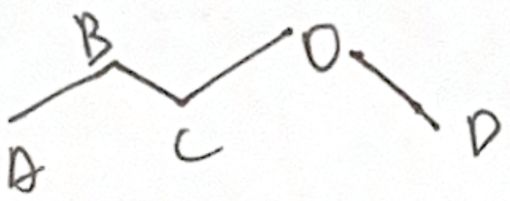
4) H_C 1H

peaks = $(\#H_A+1)\cdot(\#H_B+1)\cdot(\#\underline{CH_3}+1)$

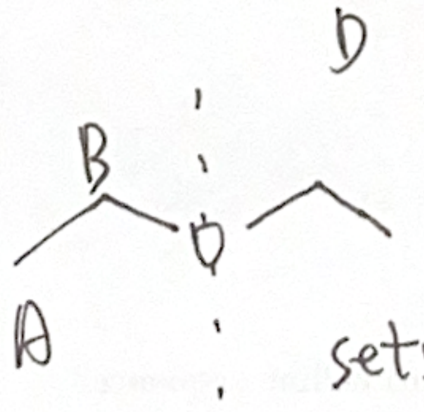
$= 2\times2\times4 = 16$ peaks



sets	Integration	splitting.
A	1H	$(\#H_B+1)\cdot(\#H_C+1)=4$
B	1H	$(\#H_A+1)\cdot(\#H_C+1)=4$
C	1H	$(\#H_A+1)\cdot(\#H_B+1)\cdot(\#H_D+1)=2\times2\times3=12$
D	2H	~~$(\#H_C+1)\cdot(\#H_E+1)=2\times4=8$~~ ? $n+1=5$.
E	3H	$n+1=2+1=3$



sets	Integration	splitting	Type of Hatom	chemical shift
A	3	$2+1=3$	$R-CH_3$	0.8-1
B	2	$3+2+1=6$	RCH_2R	1.2-1.4
C	2	$2+1=3$	RCH_2OR	3.3-4.0
D	3	$0+1=1$	$ROCH_3$	3.3-4.0



sets	Integration	splitting
A	6	$2+1=3$
B	4	$3+1=4$