Alkanes

Isomers

Constitutional

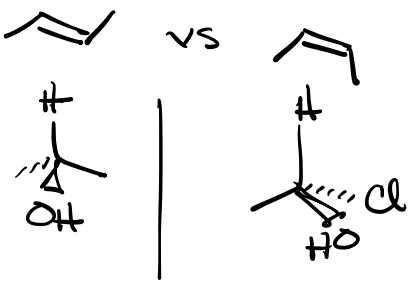
Same molecular formula but different atom connectivity

C_4H_{10}

Now

Geometric

Same molecular formula
Same atom connectivity
but different spacial arrangement



Later

Units of Unsaturation

C_nH_{2n+2} for Saturated

molecule will have no double bonds and no rings

$C_nH_{2n+2+N-X}$

N = nitrogen
X = halogen F, Cl, Br, I

Oxygen does not affect units of unsat

Loss of 2 H's = 1 unit of unsaturation

Saturated example

$C_5H_{11}Br$

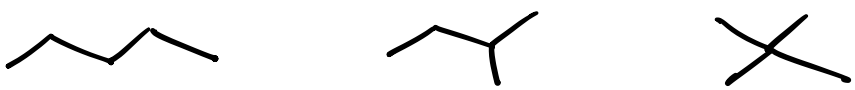
$C_nH_{2n+2+N-X}$ $\quad H_{2(5)+2+0-1}$

H_{10+2-1}

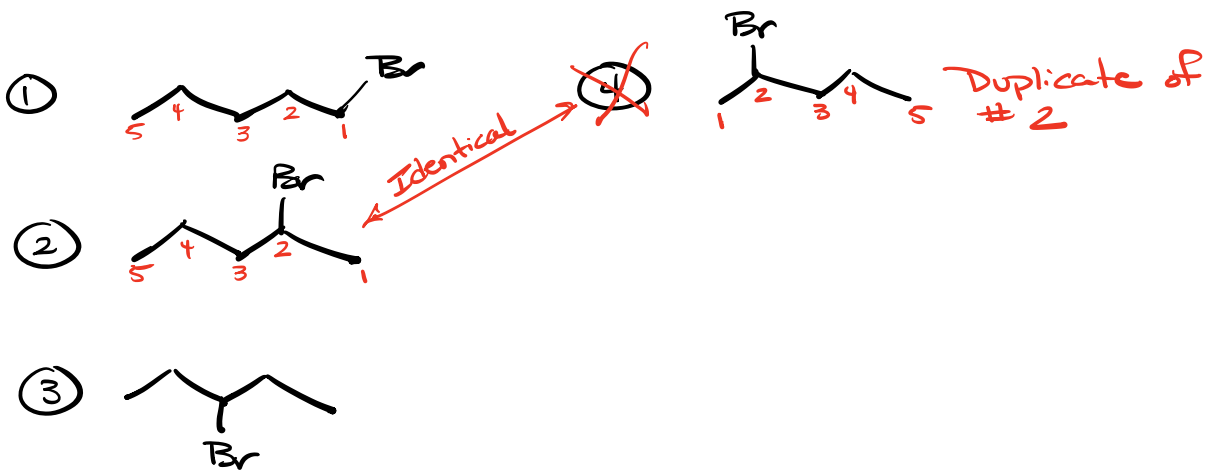
H_{11} ✓ molecule is saturated

No Rings
No Double bonds

Frame Works

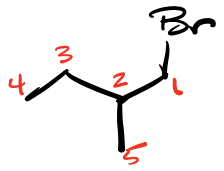


Linear 



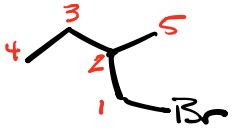
Branched

Never change orientation of framework.

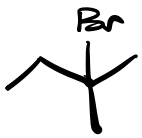
④ 

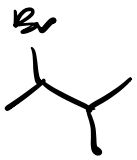
Identical

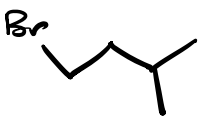
~~⑧~~



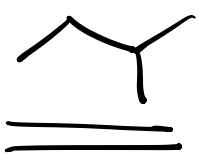
duplicate of #4

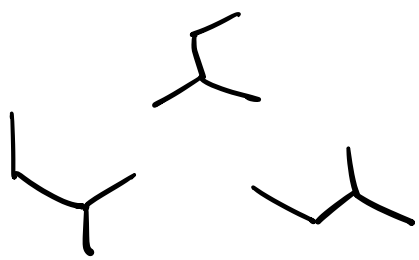
⑤ 

⑥ 

⑦ 

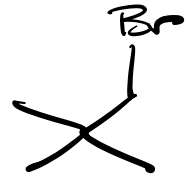
*Tip: use model kit & build both. If they can be rotated and overlap ⇒ They are the same. If you must break a bond & reconnect to get them to be the same, then the two were isomers.





Don't change orientation

Branched

(8) 

× 

Error
5 bonds
to Carbon

Total & Constitutional Isomers for $C_5H_{11}Br$

C_4H_7Br Find all of the Constitutional isomers.

$C_nH_{2n+2+N-X}$

$H_{2(4)+2+0-1}$

H_9 if Saturated

$-\ H_7$ # of hydrogens in formula

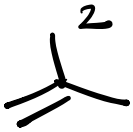
$2 \mid H_2$

1 unit of unsaturation
= Loss of 2 Hydrogens

Molecule has either 1 Ring
or 1 double bond

Frame works

Linear  5  2  2 Geometric

Branched  2

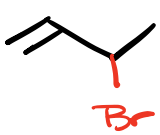
Ring  3 (5 if Geometric)  1

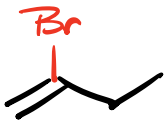
13 Constitutional

17 if we Consider Geometric Isomers

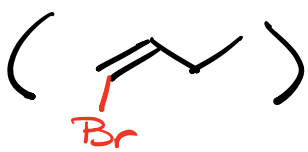
Linear C_4H_7Br

1. 

2. 

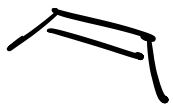
3. 

4.  trans

5.  Cis Geometric

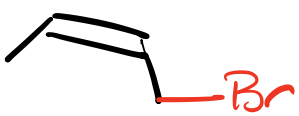
Linear

Geometric

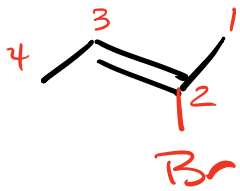


(6)

(8)

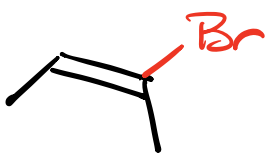


(7)



same

(9)



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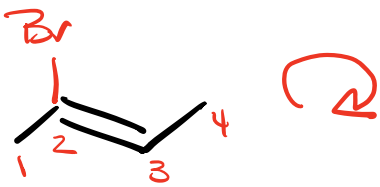
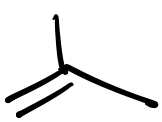
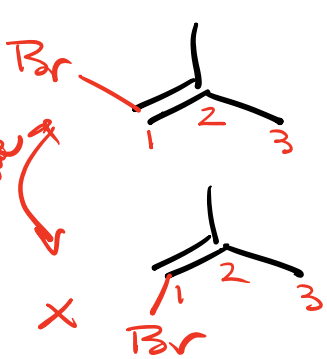


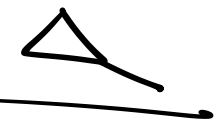
Branched



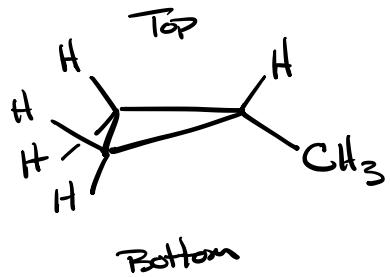
(10)

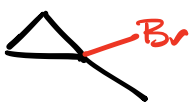
(11)



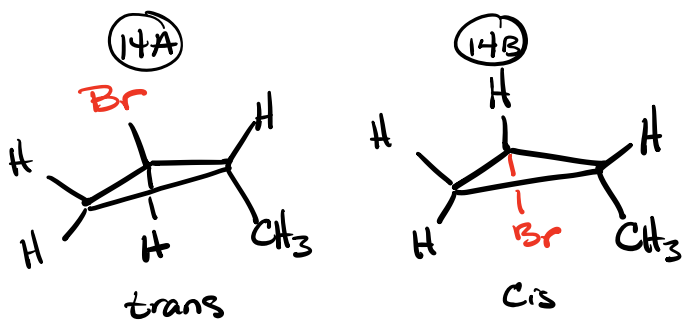
Ring 

(12) 

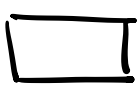


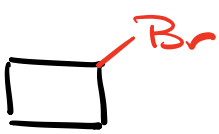
(13) 

(14) * 



Geometric

Ring 

(15) 

Drawing Isomers

① units of unsaturation
⇒ # possibilities
$C_nH_{2n+2+N-X}$

② Draw all frameworks

*③ Draw isomers from framework without rotating things

④ Watch for dublicates
⇒ Numbering
⇒ Model kit

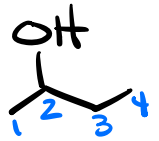
Nomenclature

Each molecule has a unique systematic name & may have 1 or more common names.

1892 IUPAC Established

1958 First IUPAC Rules published

1979, 1993, 2004 Rule Updates



	Common	Sec-butanol
	1979	2-butanol
	1993	butan-2-ol

Unbranched alkanes

#C

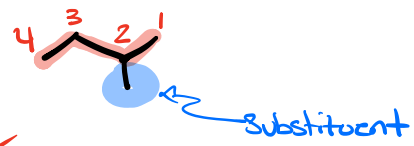
Suffix tells family or functional group

1	CH_4	methane
2	/	ethane
3	^	propane
4	~	butane
5	^^	pentane
6	~~	hexane
7	^^^	heptane
8	~~~	octane
9	^^^^	nonane
10	~~~~	decane

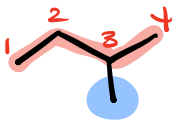
11	undecane
12	dodecane
13	tridecane
14	tetradecane
15	pentdecane
⋮	
20	icosane

Rules

1. Identify longest Carbon Chain
2. Identify Substituents
3. Number longest Carbon Chain such that the substituent at first point of difference has lowest possible #.



✓ methyl on #2
lowest #

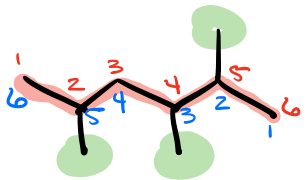


X methyl #3

4. Group identical substituents together. Locator #'s are separated by commas and followed by a dash. The name of group is preceded by a prefix indicating how many of that group are present.

5. Write name w/ substituents in alphabetical order.

Ex



First point of difference

2, 4, 5

⟹ 2, 3, 5

Blue #'s have lowest # at first point of difference

3 methyls

prefix

1 carbon

yl = Substituent

2,3,5 – trimethyl

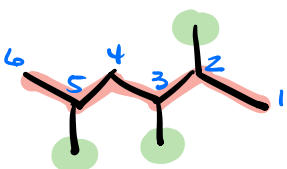
Locator positions

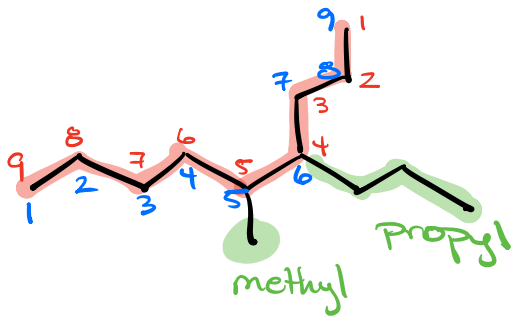
3

hexane

mon	1
di	2
tri	3
tetra	4
penta	5
hexa	6
hepta	7
octa	8
nona	9
deca	10

2,3,5 – trimethylhexane





9 Carbon Chain
nonane

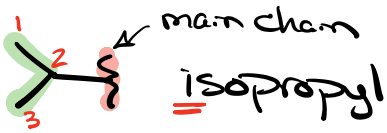
4, 5
5, 6

4-propyl
5-methyl
nonane

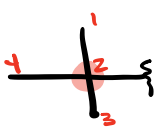
5-methyl-4-propylnonane

Complex Side chains (branched Side chains)

Common names



isopropyl

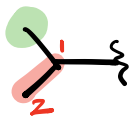


tert-butyl
tertiary

isobutyl

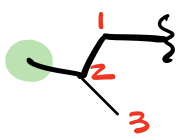
isopentyl

sec-butyl
Secondary attachment



isopropyl
(1-methylethyl)

sec-butyl
(1-methylpropyl)



isobutyl
(2-methylpropyl)