Lec 6 CHEM 30A Jan 21st

ALKANES

1. STRUCTURE
2. ISOMERS
3. NOMENCLATURE
4. CONFORMATION
5. PROPERTIES
6. CONFORMATIONAL ANALYSIS

QUIZ LOW 0/30
MEAN 18/30
HIGH 35/30

HANDED BACK IN DISCUSSION

HMK
Read 2-2.6
Problems
2.1, 2.2, 2.8, 2.9, 2.17-2.21
2.24-2.28

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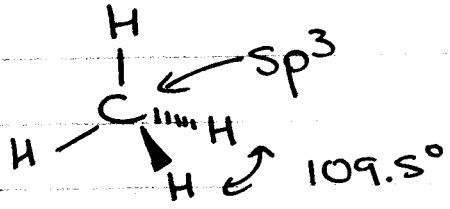
1. STRUCTURE

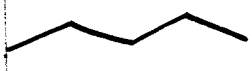
Alkanes → SATURATED HYDROCARBONS

- SATURATED → EACH C HAS MAX # H
- HYDROCARBONS → ONLY C & H

General Formula C_nH_{2n+2} (without rings)



METHANE

CH_4	methane	CH_4
CH_3-CH_3	ethane	C_2H_6
	propane	C_3H_8
	butane	C_4H_{10}
	pentane	C_5H_{12}

and so on... hex... hept... oct... non... dec...

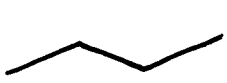
$CH_3(CH_2)_nCH_3$ UNBRANCHED

(2) ISOMERS

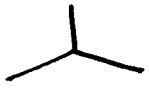
- same molecular formula, different attachment of atoms
  ⇒ CONSTITUTIONAL ISOMERS

CH_4, C_2H_6, C_3H_8 EACH HAS ONLY ONE ARRANGEMENT

HOW ABOUT C_4H_{10}



butane



2 methylpropane

Do C_6H_{14} for HMK (5 structures)

(3) NOMENCLATURE

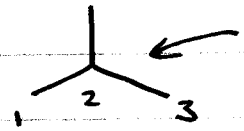
International Union of Pure and Applied Chemistry (IUPAC) ⇒ SYSTEMATIC NAMING

- STRAIGHT CHAINS (done)

- BRANCHED STRUCTURES

(i) IDENTIFY LONGEST CHAIN

(ii) EACH SUBSTITUENT GETS A NAME AND A NUMBER

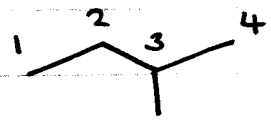


← 2-METHYL-PROPANE

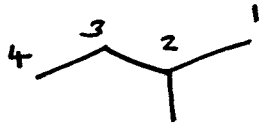
ALKYL GROUPS

CH_3- methyl
CH_3CH_2- ethyl
$CH_3CH_2CH_2-$ propyl
$CH_3CH_2CH_2CH_2-$ butyl etc, etc

(iii) MINIMIZE SUBSTITUENT NUMBER

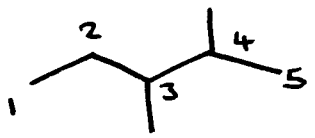


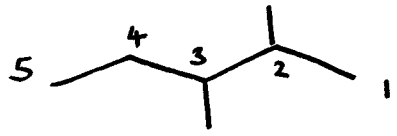
3-METHYLBUTANE ✗



2-METHYLBUTANE ✓

(iv) SAME SUBSTITUENT MORE THAN ONCE

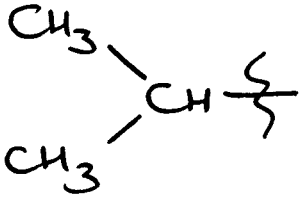




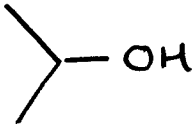
2,3 – DIMETHYL PENTANE

After this, it gets SILLY!

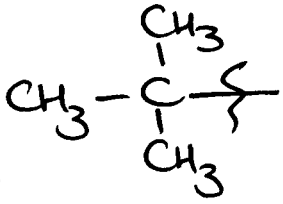
COMMON NAMES



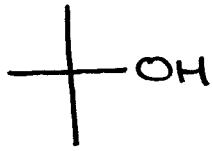
isopropyl



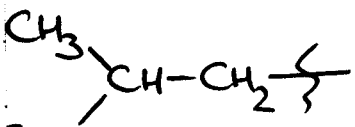
isopropyl alcohol



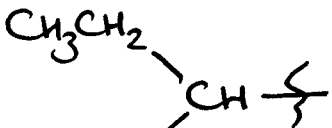
tert-butyl



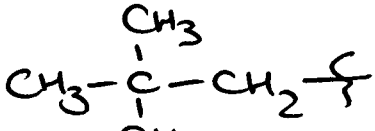
t-butyl alcohol



isobutyl



sec-butyl

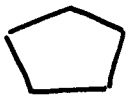


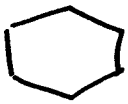
neo-pentyl

CYCLOALKANES

CYCLOPROPANE C_3H_8

 CYCLOBUTANE C_4H_8

 CYCLOPENTANE C_5H_{10}

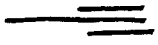
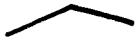
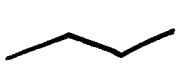
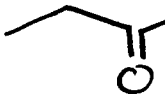
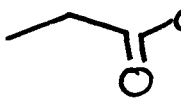
 CYCLOHEXANE C_6H_{12}

BICYCLOALKANES — FORGET IT!

General rules:

PREFIX – INFIX – SUFFIX

PROP	AN	E	
3Cs	Single Bonds	Hydrocarbons	

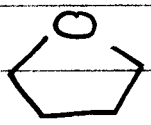
INFIX	–EN–	 PROPENE
	–YN–	 PROPYNE
SUFFIX	–E	 PROPANE
	–OL	 PROPANOL
	–AL	 PROPANAL
	–ONE	 PROPANONE
	–OIC ACID	 PROPANOIC ACID
	(–AMINE)*	 PROPYL AMINE

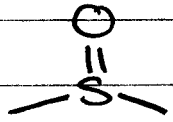
Common Structures / Names / Acronyms

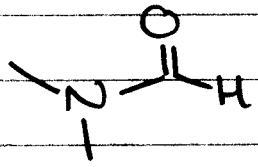
- Keep a notebook

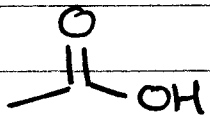
 acetone

 pyridine

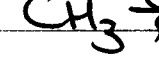
 tetrahydrofuran (THF)

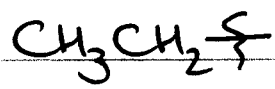
 dimethyl sulfoxide (DMSO)

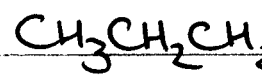
 dimethyl formamide (DMF)

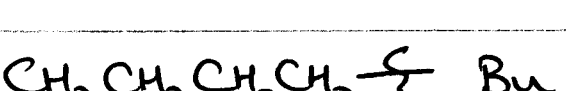
 acetic acid (AcOH)

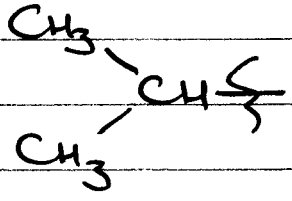
- other common abbreviations

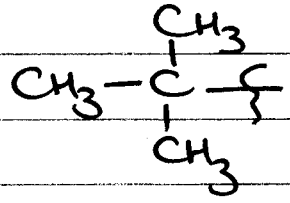
 Me

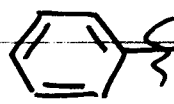
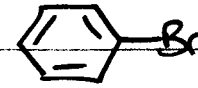
 Et

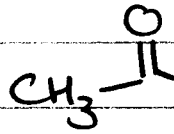
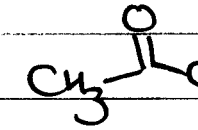
 Pr

 Bu

 ^{i}Pr

 ^{t}Bu

 Ph (PHENYL) e.g.  = PhBr

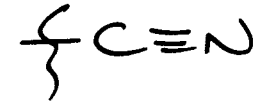
 Ac (ACETYL) e.g.  = AcCl

R GROUPS – stuff dangling off the area of interest in a molecule

e.g. R–Cl, R–OH, R–CO_2H

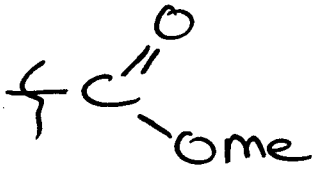
a chloride an alcohol a carboxylic acid

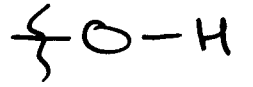
FUNCTIONAL GROUPS



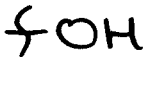
$\sim C\equiv N$

$\sim CN$



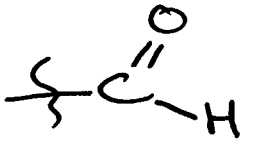


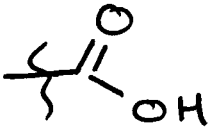
$\sim O-H$



$\sim OH$

$\sim NO_2$



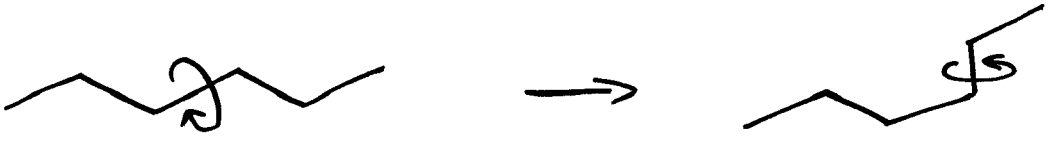


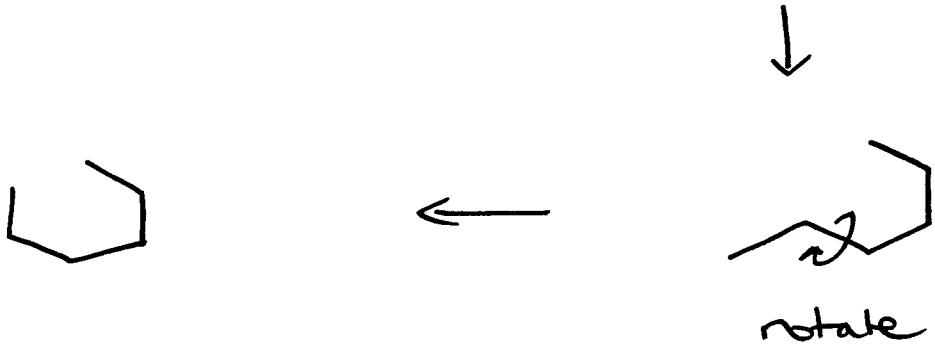
$\sim CO_2H$

$\sim CHO$

(6) CONFORMATIONAL ANALYSIS

– consider HEXANE



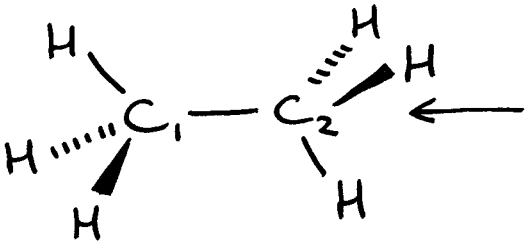


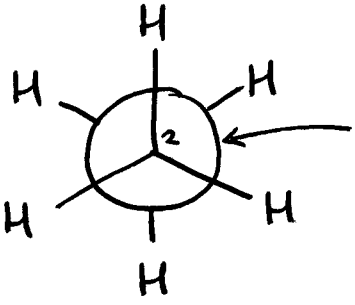
THESE ARE ALL THE SAME MOLECULE

Different arrangements of atoms that result from ONLY single bond rotations are called CONFORMATIONS

At room temperature, all single bonds are constantly rotating

consider C_2H_6





LOOK DOWN C–C BOND

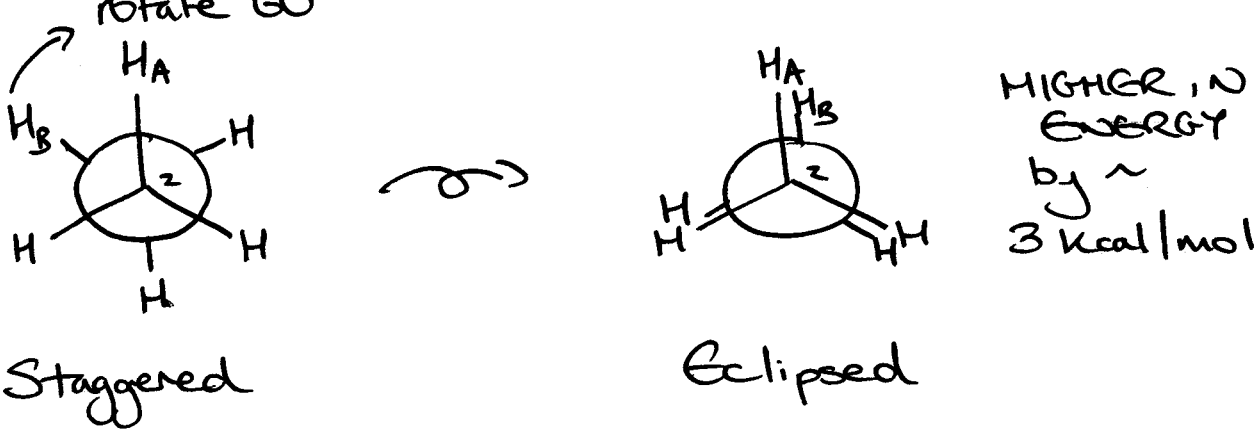
NEWMAN PROJECTION

- TWO METHYL GROUPS CAN ROTATE wrt ONE ANOTHER (0-360°)

  ⇒ INFINITE NUMBER OF CONFORMATIONS

- At RT, rate of rotation is ~10000000000 s^{-1}

However, rotation is not completely UNHINDERED



angle between 2 intersecting PLANES

$H_A C_2 C_1$ & $H_B C_1 C_2$