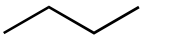
Chapter 3: Alkanes and Cycloalkanes

Alkane Structures (B&P 3.1, 3.2, 3.4)

Alkanes are **saturated hydrocarbons** (only carbon and hydrogen, and with the maximum number of hydrogens - so no pi bonds, only sigma/single bonds)

alkane formula: $\mathbf{C_nH_{2n+2}}$

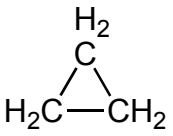
CH_4	methane	CH_4
CH_3CH_3	ethane	C_2H_6
$CH_3CH_2CH_3$	propane	C_3H_8
$CH_3(CH_2)_2CH_3$ 	butane	$C_4H\_\_$

C_5H	pentane	C_8H	octane
C_6H	hexane	C_9H	nonane
C_7H	heptane	$C_{10}H$	decane

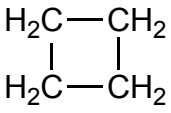
line drawing for decane:

Draw isomers (constitutional isomers) of C_5H_{12} .

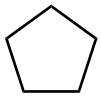
cycloalkane formula: $\mathbf{C_nH_{2n}}$

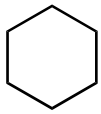


cyclopropane



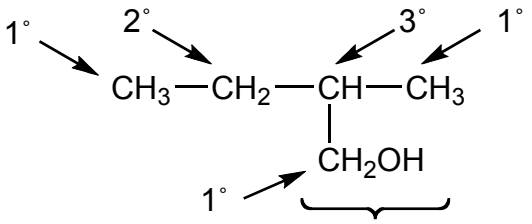
cyclobutane





Types of carbons

primary (1˚)	attached to one carbon
secondary (2˚)	attached to two carbons
tertiary (3˚)	attached to three carbons
quaternary (4˚)	attached to four carbons



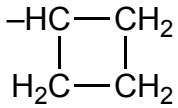
described as a primary alcohol (1˚ ROH)

IUPAC Rules for naming alkanes (B&P 3.3)

1. Find the longest carbon chain (if there is a tie, choose chain with the most substitutents). Name parent (one C = methane, two C's = ethane, three C's = propane, etc.).
2. Number the carbon chain, starting from the end closest to the first substituent.
3. Name and number the substituents (use di, tri, tetra, etc., prefixes for groups that appear more than once). Insert dashes between numbers and letters, and commas between numbers
4. Alphabetize* and list substituents before the parent name. *Ignore all prefixes other than iso.

Alkyl Substituents (R–)
(groups attached to parent)

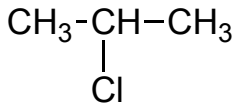
$-CH_3$	methyl (Me)
$-CH_2CH_3$	ethyl (Et)
$-CH_2CH_2CH_3$	propyl (Pr)
$-CH_2(CH_2)_2CH_3$	butyl (Bu)

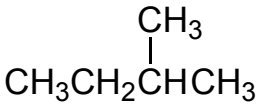


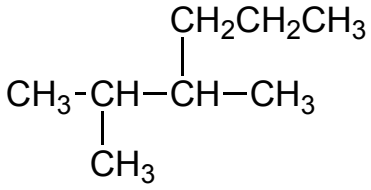
cyclobutyl

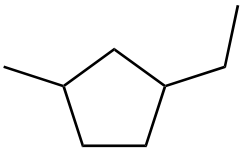
Other Substituents
(groups attached to parent)

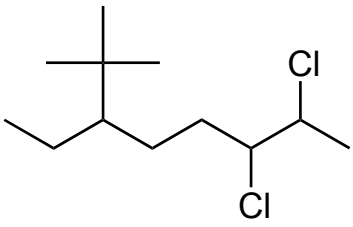
–F	fluoro
–Cl	chloro
–Br	bromo
–I	iodo









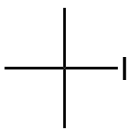


Common names for alkyl groups

$-CH_2CH_2CH_3$	*n*-propyl (*n*-Pr)
CH_3CHCH_3	isopropyl (*i*-Pr)
$-CH_2(CH_2)_2CH_3$	*n*-butyl (*n*-Bu)
$CH_3CHCH_2CH_3$	*sec*-butyl (*s*-Bu)
CH_2CHCH_3	isobutyl (*i*-Bu)
CH_3-C-CH_3	*tert*-butyl (*t*-Bu)

sec-butyl alcohol

n-propyl alcohol



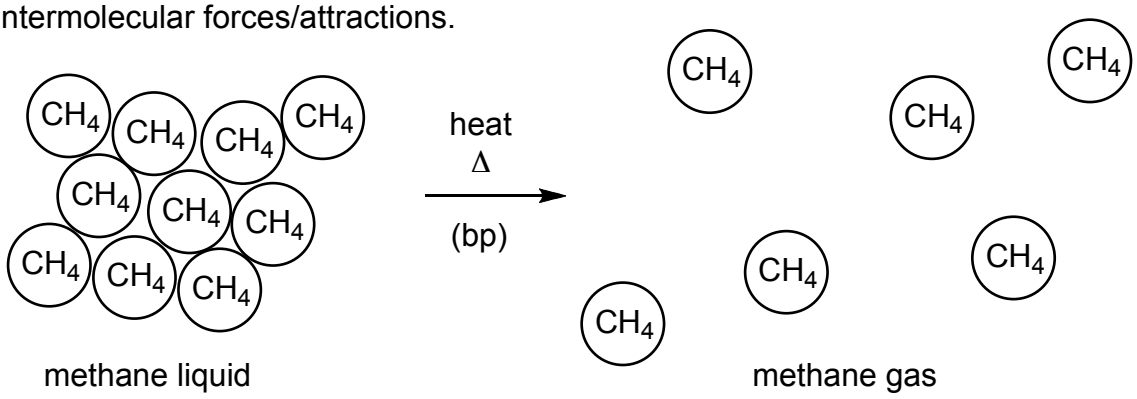
Properties of Alkanes (B&P 3.8)

- nonpolar, hydrophobic
- isolated from petroleum/crude oil (B&P 3.10)
- very stable and unreactive (all strong sigma bonds - no pi bonds or lone pairs)
  - used as fuel: combustion reaction (B&P 3.9)

$$CH_4 + 2\,O_2 \longrightarrow CO_2 + 2\,H_2O + \text{heat} \qquad \Delta H^\circ = -212 \text{ kcal/mol}$$

Predicting Relative Boiling Points (B&P 3.8)

Physical properties, such as water solubility and boiling point (bp) are based on intermolecular forces/attractions.



if CH_4 molecules are strongly attracted to one another, then

- requires a lot of energy to separate them from each other
- will have a high/low boiling point

Types of "nonbonding" interactions

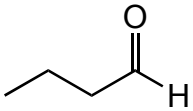
A Dipole-Dipole

B Hydrogen Bonding

C van der Waal's/London Dispersion

A Dipole-Dipole - attraction between polar molecules (consider geometry! Is CCl_4 polar?)

a polar molecule:



	NaCl		
bp ˚C	1413	76	36

Overall trend:

polarity

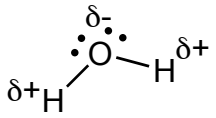
bp

B Hydrogen Bonding - strongest known dipole due to H on N or O

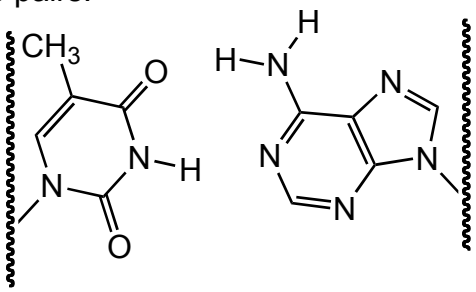
H—N H—O both are <u>extremely</u> polar bonds

	H_2O	CH_3CH_2OH	CH_3OCH_3	$CH_3CH_2CH_3$
bp ˚C	100	78	-24	-42

hydrogen-bonding in water:



hydrogen-bonding in DNA base pairs:



thymine (T) adenine (A)

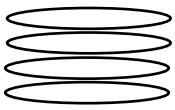
C Van der Waal's/London Dispersion Forces - induced (temporary) dipoles in nonpolar molecules

temporary attraction because of uneven distribution of electrons

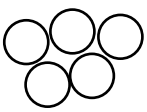
- the greater the surface area, the greater the VDW/Dispersion forces (think "Velcro")
- the higher the MW, the higher the bp (if all polarity is equal)

	$CH_3CH_2CH_2CH_3$	$CH_3-C(CH_3)_2-CH_3$	$CH_3CH_2CH_2CH_2CH_3$	$C_{31}H_{64}$
bp ˚C	-1	10	36	> 300

straight-chain vs. branched



more surface area (more contact)



less surface area (less contact)

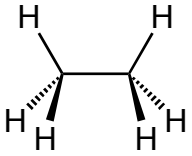
to predict boiling points

1) H-bonding (OH or NH)
2) polar vs. nonpolar
3) ⇧ MW, ⇧ bp
4) branching (least important!)

Conformations of Alkanes (B&P 3.6)

conformers - structures that differ only by rotation about single/sigma (σ) bonds

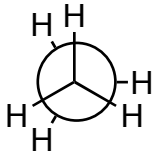
Ethane



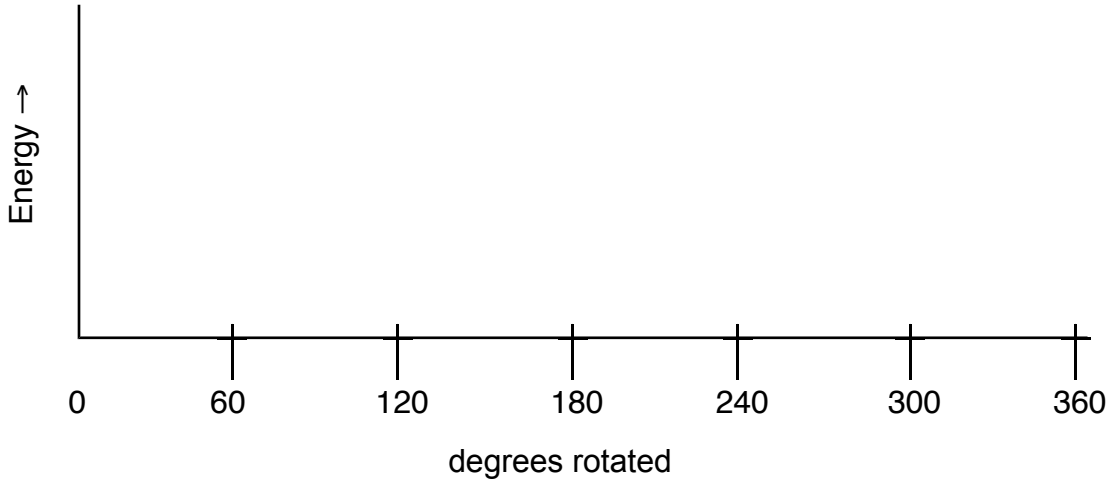
60˚ rotation ⇌

rapidly interconverting conformers

Newman Projection



60˚ rotation ⇌



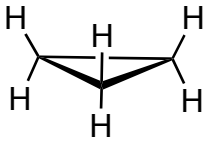
Conformations of Butane

$CH_3-CH_2-CH_2-CH_3$

Structure and Conformations of Cycloalkanes (B&P 3.4, 3.6)

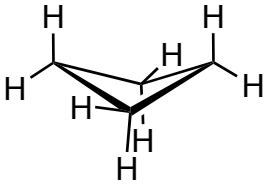
cyclopropane

cyclobutane



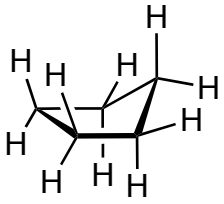
- sp^3 bond angle can't be 109.5˚

- eclipsing H's



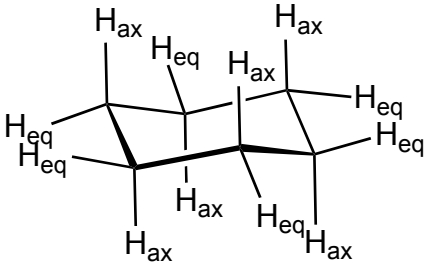
** these small rings have a large amount of "ring strain" **

cyclopentane
- has very little ring strain



the envelope conformation

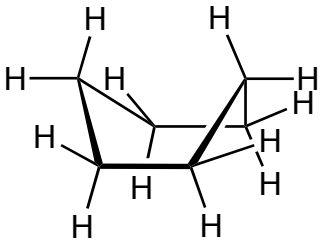
cyclohexane
- has NO ring strain!
- six-membered rings are commonly found in nature



chair conformation

H_{ax} = axial position
(straight up or down)

H_{eq} = equatorial position
(slightly up or down)



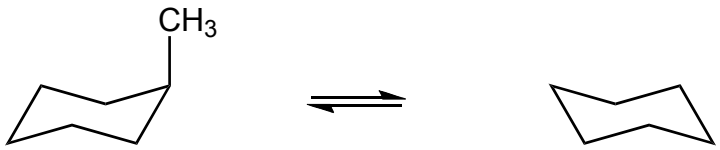
boat conformation

drawing a chair:

opposite sides
are parallel

Need more help?
See cyclohexane
playlist on YouTube!

Draw and compare stabilities of the two chair conformations of methylcyclohexane (chair "flip").



Draw the two chairs of *cis*-1-*t*-butyl-4-methylcyclohexane. Which is more stable? (B&P 3.7)

Suggested Problems:
see CHM 201 course homepage

Extra credit (+1 point on Exam I):
Do the Ch 1-3 "Putting it Together" problems 1-19 (but skip 14e, 15 and 16). Exchange your work with a classmate and grade with red ink (or self correct). Turn in "graded" work.