

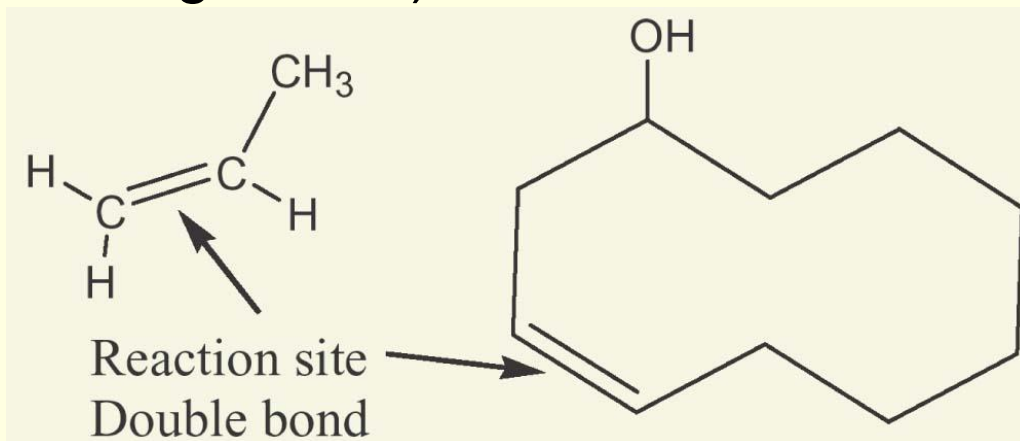
Alkanes and Cycloalkanes

Families of Organic Compounds

- Organic compounds can be grouped into families by their common structural features
- We shall survey the nature of the compounds in a tour of the families in this course
- This chapter deals with *alkanes*, compounds that contain only carbons and hydrogens, all connected exclusively by single bonds

Functional Groups

- **Functional group** - collection of atoms at a site within a molecule with a common bonding pattern
- The group reacts in a typical way, generally independent of the rest of the molecule
- For example, the double bonds in simple and complex alkenes react with bromine in the same way (See Figure 3.1)

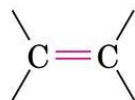
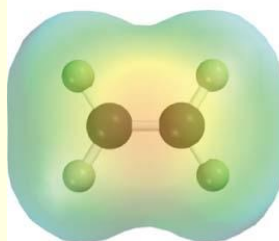


Survey of Functional Groups

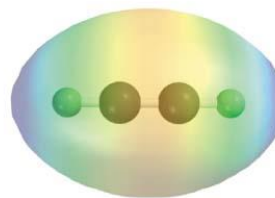
- Table 3.1 lists a wide variety of functional groups that you should recognize
- As you learn about them in each chapter it will be easier to recognize them
- The functional groups affect the reactions, structure, and physical properties of every compound in which they occur

Types of Functional Groups: Multiple Carbon–Carbon Bonds

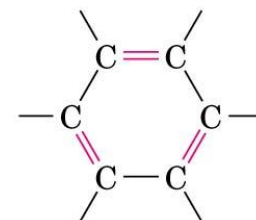
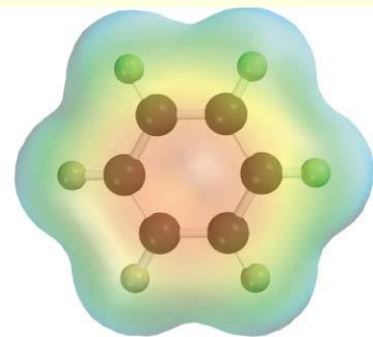
- *Alkenes* have a C-C double bond
- *Alkynes* have a C-C triple bond
- *Arenes* have special bonds that are represented as alternating single and double C-C bonds in a six-membered ring



Alkene



Alkyne



**Arene
(aromatic ring)**

Functional Groups with Carbon Singly Bonded to an Electronegative Atom

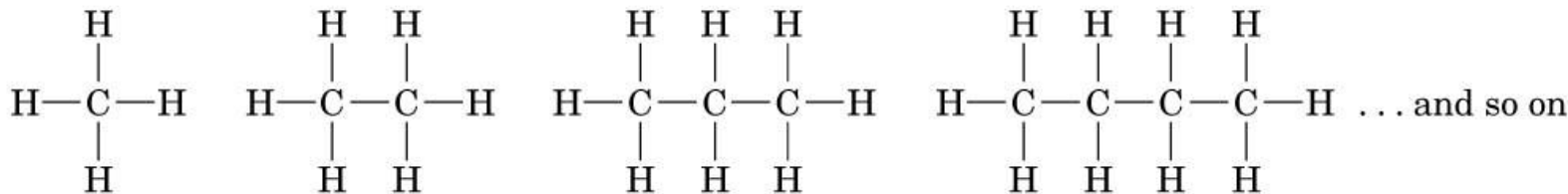
- *Alkyl halide*: C bonded to halogen (C-X)
- *Alcohol*: C bonded O of a hydroxyl group (C-OH)
- *Ether*: Two C's bonded to the same O (C-O-C)
- *Amine*: C bonded to N (C-N)
- *Thiol*: C bonded to SH group (C-SH)
- *Sulfide*: Two C's bonded to same S (C-S-C)
- Bonds are polar, with partial positive charge on C ($\delta+$) and partial negative charge ($\delta-$) on electronegative atom

Groups with a Carbon–Oxygen Double Bond (Carbonyl Groups)

- *Aldehyde*: one hydrogen bonded to C=O
- *Ketone*: two C's bonded to the C=O
- *Carboxylic acid*: —OH bonded to the C=O
- *Ester*: C-O bonded to the C=O
- *Amide*: C-N bonded to the C=O
- *Acid chloride*: Cl bonded to the C=O
- Carbonyl C has partial positive charge ($\delta+$)
- Carbonyl O has partial negative charge ($\delta-$).

Alkanes and Alkane Isomers

- Alkanes: Compounds with C-C single bonds and C-H bonds only (no functional groups)
- Connecting carbons can lead to large or small molecules
- The formula for an alkane with no rings in it must be C_nH_{2n+2} where the number of C's is n
- Alkanes are **saturated** with hydrogen (no more can be added)
- They are also called **aliphatic compounds**



Methane

Ethane

Propane

Butane

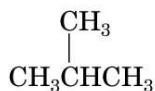
Alkane Isomers

- CH_4 = methane, C_2H_6 = ethane, C_3H_8 = propane
- The molecular formula of an alkane with more than three carbons can give more than one structure
 - C_4 (butane) = butane and isobutane
 - C_5 (pentane) = pentane, 2-methylbutane, and 2,2-dimethylpropane
- Alkanes with C's connected to no more than 2 other C's are **straight-chain** or **normal alkanes**
- Alkanes with one or more C's connected to 3 or 4 C's are **branched-chain alkanes**

Constitutional Isomers

- Isomers that differ in how their atoms are arranged in chains are called **constitutional isomers**
- Compounds other than alkanes can be **constitutional isomers** of one another
- They must have the same molecular formula to be isomers

Different carbon skeletons
 C_4H_{10}



and



2-Methylpropane
(Isobutane)

Butane

Different functional groups
 C_2H_6O



and



Ethyl alcohol

Dimethyl ether

Different position of functional groups
 C_3H_9N



and

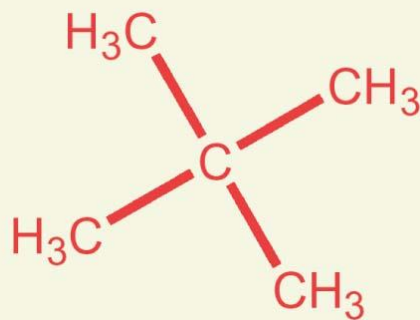
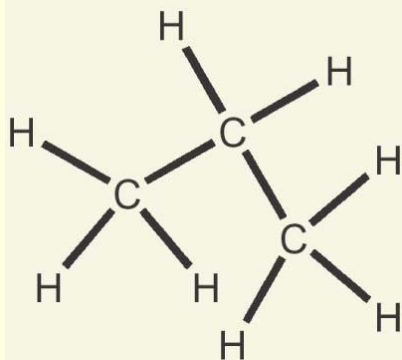


Isopropylamine

Propylamine

Condensed Structures of Alkanes

- We can represent an alkane in a brief form or in many types of extended form
- A condensed structure does not show bonds but lists atoms, such as
 - $\text{CH}_3\text{CH}_2\text{CH}_3$ (propane)
 - $\text{CH}_3(\text{CH}_2)_2\text{CH}_3$ (2,2-dimethylpropane)



Names of Small Hydrocarbons

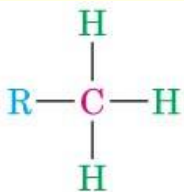
No. of Carbons	Formula Name	(C_nH_{2n+2})
1	Methane	CH_4
2	Ethane	C_2H_6
3	Propane	C_3H_8
4	Butane	C_4H_{10}
5	Pentane	C_5H_{12}
6	Hexane	C_6H_{14}
7	Heptane	C_7H_{16}
8	Octane	C_8H_{18}
9	Nonane	C_9H_{20}
10	Decane	$C_{10}H_{22}$

3.3 Alkyl Groups

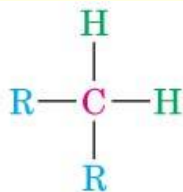
- **Alkyl group** – remove one H from an alkane (a part of a structure)
- General abbreviation “R” (for Radical, an incomplete species or the “rest” of the molecule)
- Name: replace *-ane* ending of alkane with *-yl* ending
 - $\square\text{CH}_3$ is “methyl” (from methane)
 - $\square\text{CH}_2\text{CH}_3$ is “ethyl” from ethane
- See Table 3.4 for a list

Types of Alkyl groups

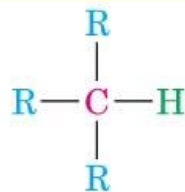
- Classified by the connection site (See Figure 3.3)
 - a carbon at the end of a chain (primary alkyl group)
 - a carbon in the middle of a chain (secondary alkyl group)
 - a carbon with three carbons attached to it (tertiary alkyl group)



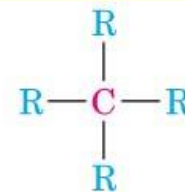
Primary carbon (1 γ)
is bonded to one
other carbon
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Secondary carbon (2 γ)
is bonded to two
other carbons



Tertiary carbon (3 γ)
is bonded to three
other carbons



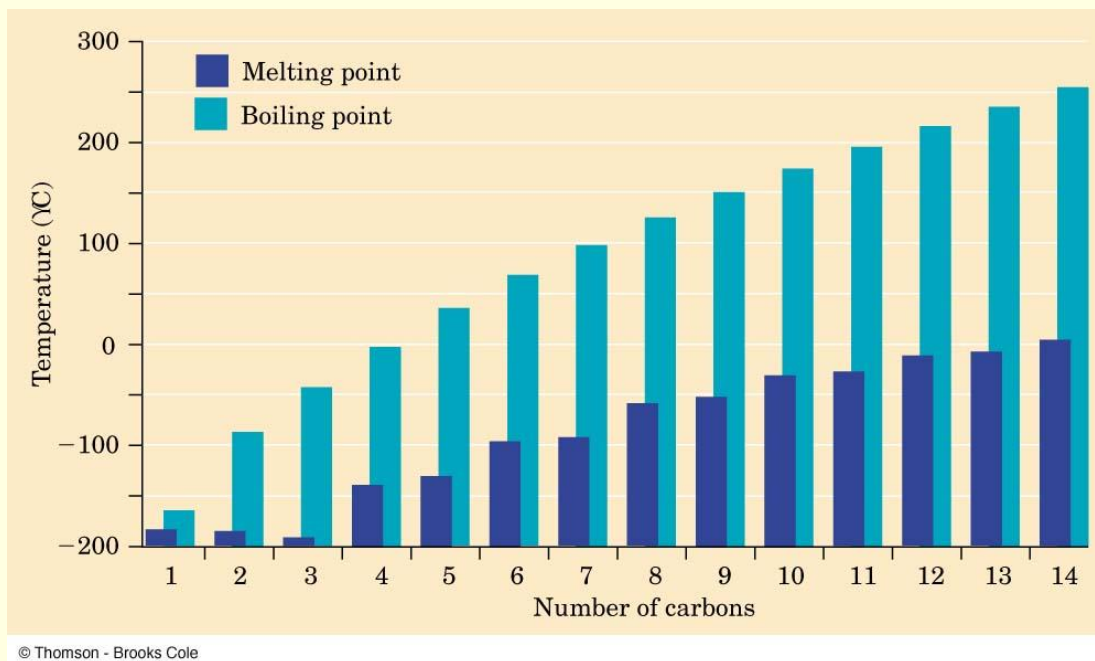
Quaternary carbon (4 γ)
is bonded to four
other carbons

Naming Alkanes

- Compounds are given systematic names by a process that uses
 - Prefix-Parent-Suffix
- Follows specific rules
 - Named as longest possible chain
 - Carbons in that chain are numbered in sequence
 - substituents are numbered at their point of attachment
 - Compound name is one word (German style)
 - Complex substituents are named as compounds would be
- See specific examples in text

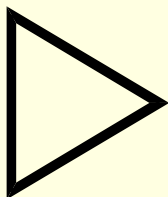
Physical Properties

- Boiling points and melting points increase as size of alkane increases
- Forces between molecules (temporary dipoles, dispersion) are weak

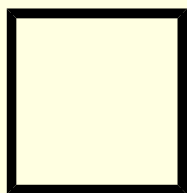


3.6 Cycloalkanes

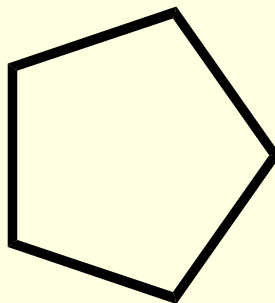
- **Cycloalkanes** are alkanes that have carbon atoms that form a ring (called alicyclic compounds)
- Simple cycloalkanes rings of —CH₂— units, (CH₂)_n, or C_nH_{2n}
- Structure is shown as a regular polygon with the number of vertices equal to the number of C's (a projection of the actual structure)



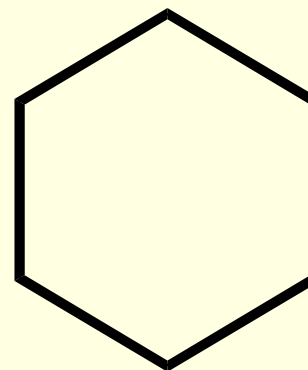
cyclopropane



cyclobutane



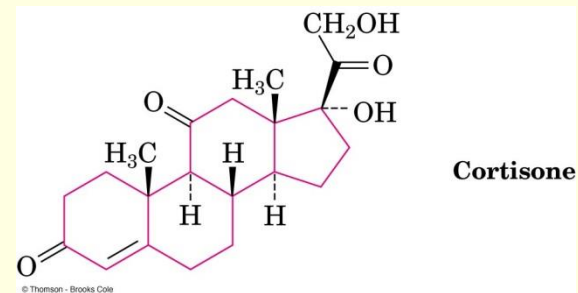
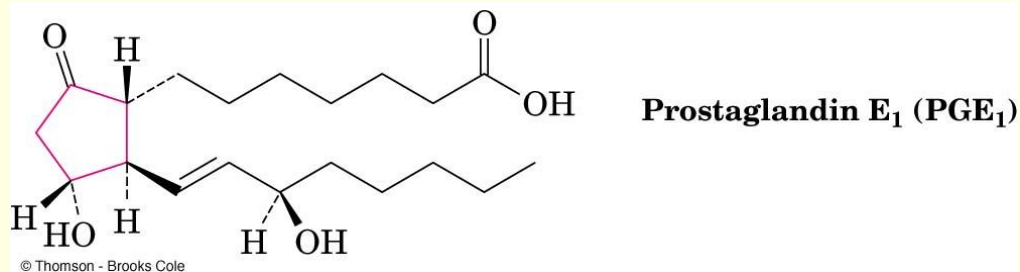
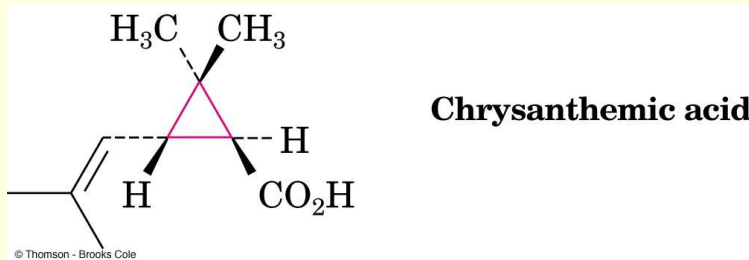
cyclopentane



cyclohexane

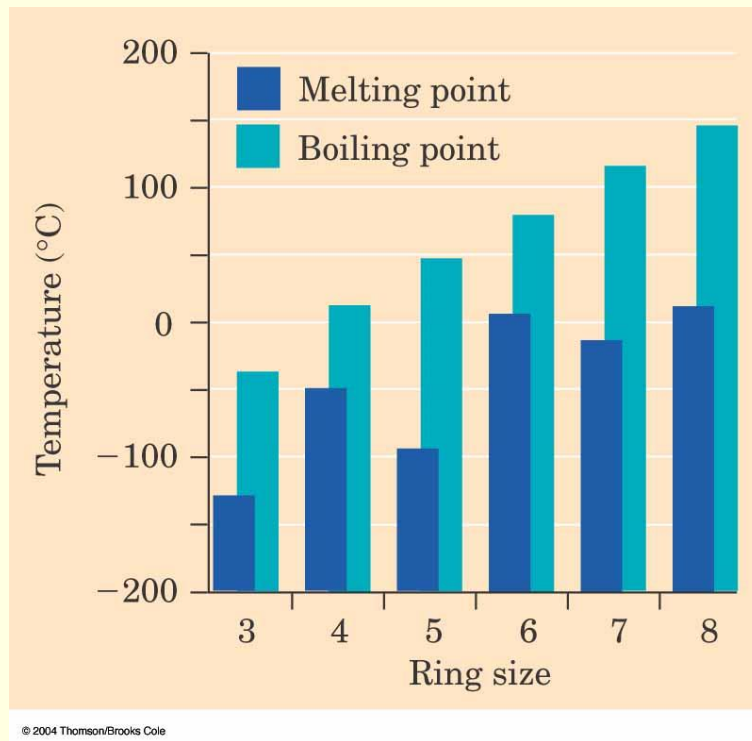
Complex Cycloalkanes

- Naturally occurring materials contain cycloalkane structures
- Examples: chrysanthemic acid (cyclopropane), prostaglandins (cyclopentane), steroids (cyclohexanes and cyclopentane)



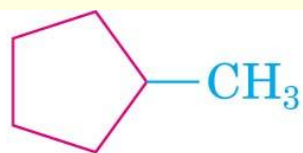
Properties of Cycloalkanes

- Melting points are affected by the shapes and the way that crystals pack so they do not change uniformly

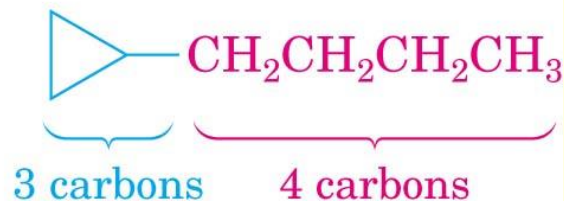


Naming Cycloalkanes

- Count the number of carbon atoms in the ring and the number in the largest substituent chain. If the number of carbon atoms in the ring is equal to or greater than the number in the substituent, the compound is named as an alkyl-substituted cycloalkane
- For an alkyl- or halo-substituted cycloalkane, start at a point of attachment as C1 and number the substituents on the ring so that the *second* substituent has as low a number as possible.
- Number the substituents and write the name
- See text for more details and examples



BUT



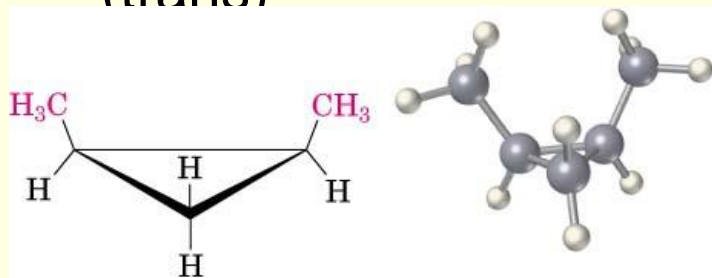
Methylcyclopentane

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1-Cyclopropylbutane

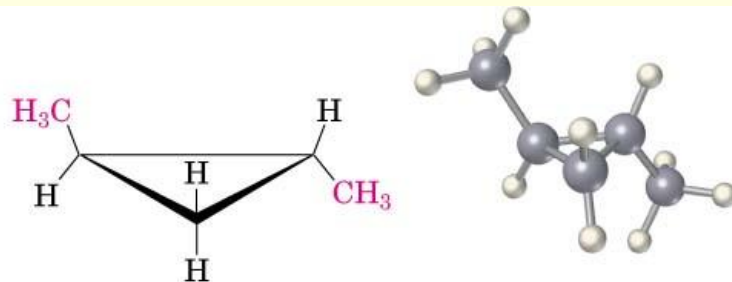
3.8 Cis-Trans Isomerism in Cycloalkanes

- Rotation about C-C bonds in cycloalkanes is limited by the ring structure
- Rings have two “faces” and substituents are labeled as to their relative facial positions
- There are two different 1,2-dimethyl-cyclopropane isomers, one with the two methyls on the same side (cis) of the ring and one with the methyls on opposite sides (trans)



cis-1,2-Dimethylcyclopropane

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trans-1,2-Dimethylcyclopropane

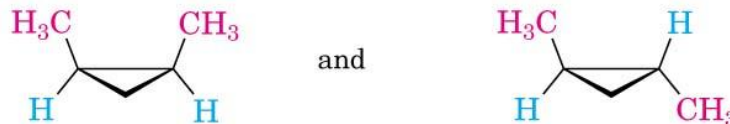
Stereoisomers

- Compounds with atoms connected in the same order but which differ in three-dimensional orientation, are **stereoisomers**
- The terms “cis” and “trans” should be used to specify stereoisomeric ring structures
- Recall that **constitutional isomers** have atoms connected in different order

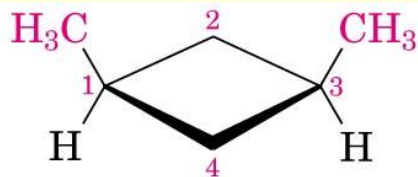
Constitutional isomers
(different connections
between atoms)



Stereoisomers
(same connections
but different three-
dimensional geometry)

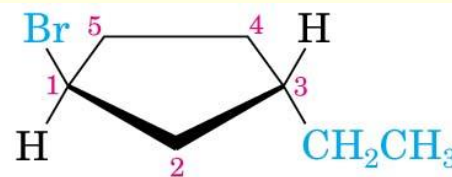


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cis-1,3-Dimethylcyclobutane

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trans-1-Bromo-3-ethylcyclopentane