CHAPTER 20: ALKANES AND ALKYL HALIDES

Organic and Biochemistry Supplement to Enhanced Introductory College Chemistry

by Gregory Anderson; Jen Booth; Caryn Fahey; Adrienne Richards; Samantha Sullivan Sauer; and David Wegman

Chapter 20 Contents

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In this chapter, you will learn about:

- Characteristics of alkanes
- Alkane formulas
- Isomers of alkanes and nomenclature
- Cycloalkanes
- Alkyl halides
- Reactions of alkanes

To better support your learning, you should be familiar with the following concepts before starting this chapter:

- Covalent Bonding (from Chapter 11: Chemical Bonding)
- Molecular structure and VSEPR (from Chapter 11: Chemical Bonding)
- General concepts of organic chemistry (from Chapter 19: Organic Chemistry)

As you just learned, there is a wide variety of organic compounds containing different functional groups. However, all organic compounds are hydrocarbons, they contain hydrogen and carbon. The general rule for hydrocarbons is that any carbon must be bonded to at least one other carbon atom, except in the case of methane which only contains one carbon. The bonded carbons form the *backbone* of the molecule to which the hydrogen atoms (or other functional groups) are attached. Refer to Appendix A: Key Element Information for more details about carbon.

Hydrocarbons with only carbon-to-carbon single bonds (C–C) are called alkanes (or saturated hydrocarbons). *Saturated*, in this case, means that each carbon atom is bonded to four other atoms (hydrogen or carbon)—the most possible; there are no double or triple bonds in these molecules.

Saturated fats and oils are organic molecules that do not have carbon-to-carbon double bonds (C=C).

The three simplest alkanes—methane (CH_4), ethane (C_2H_6), and propane (C_3H_8) shown in Figure 20.0a., are the beginning of a series of compounds in which any two members in a sequence differ by one carbon atom and two hydrogen atoms—namely, a CH_2 unit (called methylene). Alkanes follow the general formula: C_nH_{2n+2}. Using this formula, we can write a molecular formula for any alkane with a given number of carbon atoms. For example, an alkane with eight carbon atoms has the molecular formula $C_8H_{(2 \times 8) + 2} = C_8H_{18}$.

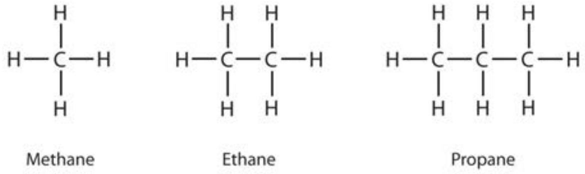


Figure 20.0a. The Three Simplest Alkanes (credit: *Intro Chem: GOB (V. 1.0).* ,CC BY-NC-SA 3.0.)

An Alkane Basis for Properties of Other Compounds

An understanding of the physical properties of the alkanes is important in that petroleum and natural gas and the many products derived from them—gasoline, bottled gas, solvents, plastics, and more—are composed primarily of alkanes. This understanding is also vital because it is the basis for describing the properties of other organic and biological compound families. For example, large portions of the structures of lipids consist of nonpolar alkyl groups as shown in Figure 20.0b. Lipids include the dietary fats and fatlike compounds called phospholipids and sphingolipids that serve as structural components of living tissues. These compounds have both polar and nonpolar groups, enabling them to bridge the gap between water-soluble and water-insoluble phases. This characteristic is essential for the selective permeability of cell membranes.

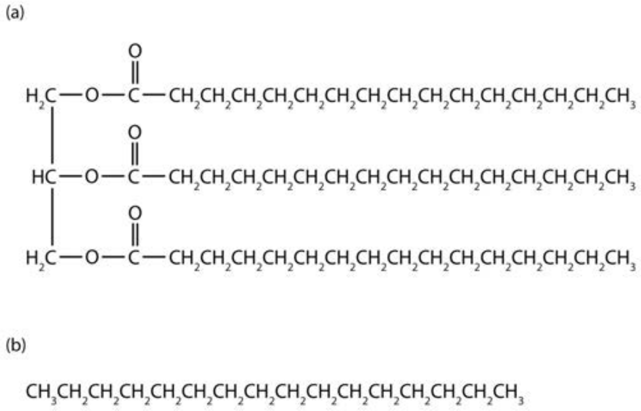


Figure 20.0b. Tripalmitin (a), a typical fat molecule, has long hydrocarbon chains typical of most lipids. Compare these chains to hexadecane (b), an alkane with 16 carbon atoms (credit: *Intro Chem: GOB (V. 1.0).* ,CC BY-NC-SA 3.0).

Attribution & References

Except where otherwise noted, this page is adapted by Adrienne Richards from “12.7: Properties of Alkanes” & “12.3: The Structure of Organic Molecules – Alkanes and Their Isomers” In *Map: Fundamentals of General Organic and Biological Chemistry (McMurry et al.)* by LibreTexts, CC BY-NC-SA 3.0 . / A derivative of “12.6: Physical Properties of Alkanes“, “12.2: Structures and Names of Alkanes“, and “12.3: Branched-Chain Alkanes” In *Basics of General, Organic, and Biological Chemistry (Ball et al.),* CC BY-NC-SA 4.0, which is a LibreTexts version of *Introduction to Chemistry: GOB (v. 1.0),* CC BY-NC 3.0.

20.1 CHARACTERISTICS OF ALKANES

Learning Objectives

By the end of this section, you will be able to:

- Understand carbon-hydrogen bonding
- Identify and name simple (straight-chain) alkanes given formulas and write formulas for straight-chain alkanes given their names.
- Identify the physical properties of alkanes and describe trends in these properties.

Alkanes

We begin our study of organic chemistry with the hydrocarbons, the simplest organic compounds, which are composed of carbon and hydrogen atoms only. As we noted, there are several different kinds of hydrocarbons. They are distinguished by the types of bonding between carbon atoms and the properties that result from that bonding.

The bonding in the hydrogen molecule is fairly straightforward, but the situation is more complicated in organic molecules with tetravalent carbon atoms. Take methane, CH_4, for instance. As we've seen, carbon has four valence electrons ($2s^2\ 2p^2$) and forms four bonds. Because carbon uses two kinds of orbitals for bonding, $2s$ and $2p$, we might expect methane to have two kinds of C–H bonds. In fact, though, all four C–H bonds in methane are identical and are spatially oriented toward the corners of a regular tetrahedron as shown in Figure 20.1a. How can we explain this?

Two regular tetrahedrons (one with 3 D representation), the wedge-bond structure, and ball and stick model of a tetrahedral carbon atom.

Figure 20.1a. A representation of van't Hoff's tetrahedral carbon atom. The solid lines represent bonds in the plane of the paper, the heavy wedged line represents a bond coming out of the plane of the page toward the viewer, and the dashed line represents a bond going back behind the plane of the page away from the viewer (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0).

An answer was provided in 1931 by Linus Pauling, who showed mathematically how an *s* orbital and three *p* orbitals on an atom can combine, or *hybridize,* to form four equivalent atomic orbitals with tetrahedral orientation. Shown in Figure 20.1b., these tetrahedrally oriented orbitals are called sp^3 hybrid orbitals. Note that the superscript 3 in the name sp^3 tells how many of each type of atomic orbital combine to form the hybrid, not how many electrons occupy it.

The 2s orbital with 2px, 2py, and 2pz orbitals undergoes hybridization to form four s p 3 orbitals oriented tetrahedrally.

Figure 20.1b. Four *sp*^{3} hybrid orbitals, oriented toward the corners of a regular tetrahedron, are formed by the combination of an *s* orbital and three *p* orbitals (red/blue). The *sp*^{3} hybrids have two lobes and are unsymmetrical about the nucleus, giving them a directionality and allowing them to form strong bonds to other atoms (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0).

The concept of hybridization explains how carbon forms four equivalent tetrahedral bonds but not why it does so. The shape of the hybrid orbital suggests the answer to why. When an *s* orbital hybridizes with three *p* orbitals, the resultant *sp*^{3} hybrid orbitals are unsymmetrical about the nucleus. One of the two lobes is larger than the other and can therefore overlap more effectively with an orbital from another atom to form a bond. As a result, *sp*^{3} hybrid orbitals form stronger bonds than do unhybridized *s* or *p* orbitals.

The asymmetry of *sp*^{3} orbitals arises because, as noted previously, the two lobes of a *p* orbital have different algebraic signs, + and –, in the wave function. Thus, when a *p* orbital hybridizes with an *s* orbital, the positive *p* lobe adds to the *s* orbital but the negative *p* lobe subtracts from the *s* orbital. The resultant hybrid orbital is therefore unsymmetrical about the nucleus and is strongly oriented in one direction.

When each of the four identical *sp*^{3} hybrid orbitals of a carbon atom overlaps with the 1*s* orbital of a hydrogen atom, four identical C–H bonds are formed and methane results. Each C–H bond in methane has a strength of 439 kJ/mol (105 kcal/mol) and a length of 109 pm. Because the four bonds have a specific geometry, we also can define a property called the bond angle. The angle formed by each H–C–H is 109.5°, the so-called tetrahedral angle. Methane thus has the structure shown in Figure 20.1c.

The space-filling model, wedge-dash structure, and ball and stick model of methane. The bond length between C-H is 109 pm, and the bond angle of H-C-H is 109.5 degrees.

Figure 20.1c. The structure of methane, showing its 109.5° bond angles. (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0).

The flat representations shown do not accurately portray bond angles or molecular geometry. Methane has a tetrahedral shape that chemists often portray with wedges indicating bonds coming out toward you and dashed lines indicating bonds that go back away from you. An ordinary solid line indicates a bond in the plane of the page. Recall that the VSEPR theory correctly predicts a tetrahedral shape for the methane molecule (Figure 20.1d.).

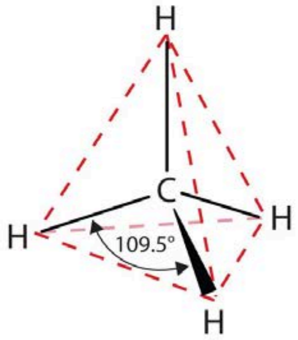


Figure 20.1d. The Tetrahedral Methane Molecule (credit: *Intro Chemistry: GOB (V. 1.0).*, CC BY-NC-SA 4.0).

Exercise 20.1a

By using the PhET Interactive Simulation, view the CH_4 molecule by selecting the Real Molecules option. From the drop-down menu, select the compound CH_4 then select Show Lone Pairs, Bond Angles, Electron Geometry, and Molecular Geometry. Alternatively, you can build your own CH_4 molecule by selecting the Model option.

Practice using the following PhET simulation: Molecule Shapes [New tab] (https://phet.colorado.edu/en/simulations/molecule-shapes)

Hydrocarbons with only carbon-to-carbon single bonds (C–C) and existing as a continuous chain of carbon atoms also bonded to hydrogen atoms are called alkanes (or saturated hydrocarbons). *Saturated*, in this case, means that each carbon atom is bonded to four other atoms (hydrogen or carbon)—the most possible; there are no double or triple bonds in the molecules. The word *saturated* has the same meaning for hydrocarbons as it does for the dietary fats and oils: the molecule has no carbon-to-carbon double bonds (C=C).

The three simplest alkanes—methane (CH_4), ethane (C_2H_6), and propane (C_3H_8) and they are shown in Figure 20.1e.

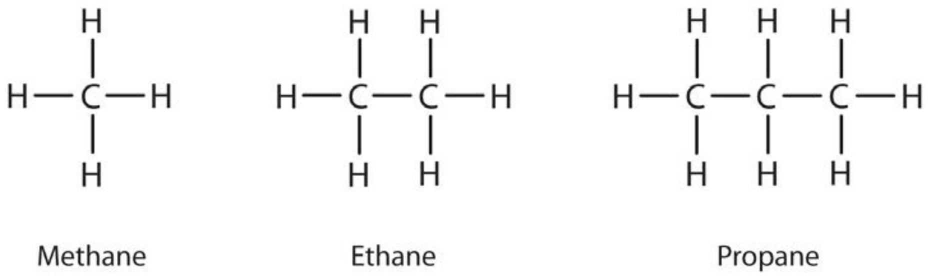


Figure 20.1e. The Three Simplest Alkanes (credit: *Intro Chemistry: GOB (V. 1.0).*, CC BY-NC-SA 4.0).

Methane (CH_4), ethane (C_2H_6), and propane (C_3H_8) are the beginning of a series of compounds in which any two members in a sequence differ by one carbon atom and two hydrogen atoms—namely, a CH_2 unit. The first 10 members of this series are given in Table 20.1a.

Table 20.1a. The First 10 Straight-Chain Alkane Formulas

Name	Molecular Formula (C_nH_{2n+2})	Condensed Structural Formula
methane	CH_4	CH_4
ethane	C_2H_6	CH_3CH_3
propane	C_3H_8	$CH_3CH_2CH_3$
butane	C_4H_{10}	$CH_3CH_2CH_2CH_3$
pentane	C_5H_{12}	$CH_3CH_2CH_2CH_2CH_3$
hexane	C_6H_{14}	$CH_3CH_2CH_2CH_2CH_2CH_3$
heptane	C_7H_{16}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$
octane	C_8H_{18}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
nonane	C_9H_{20}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
decane	$C_{10}H_{22}$	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$

Table source: “12.2: Structures and Names of Alkanes” In *Basics of GOB Chemistry (Ball et al.)*, CC BY-NC-SA 4.0.

Consider the series in Figure 20.1f. The sequence starts with C_3H_8, and a CH_2 unit is added in each step moving up the series. Any family of compounds in which adjacent members differ from each other by a definite factor (here a CH_2 group) is called a homologous series. The members of such a series, called *homologs*, have properties that vary in a regular and predictable manner. The principle of *homology* gives organization to organic chemistry in much the same way that the periodic table gives organization to inorganic chemistry. Instead of a bewildering array of individual carbon compounds, we can study a few members of a homologous series and from them deduce some of the properties of other compounds in the series.

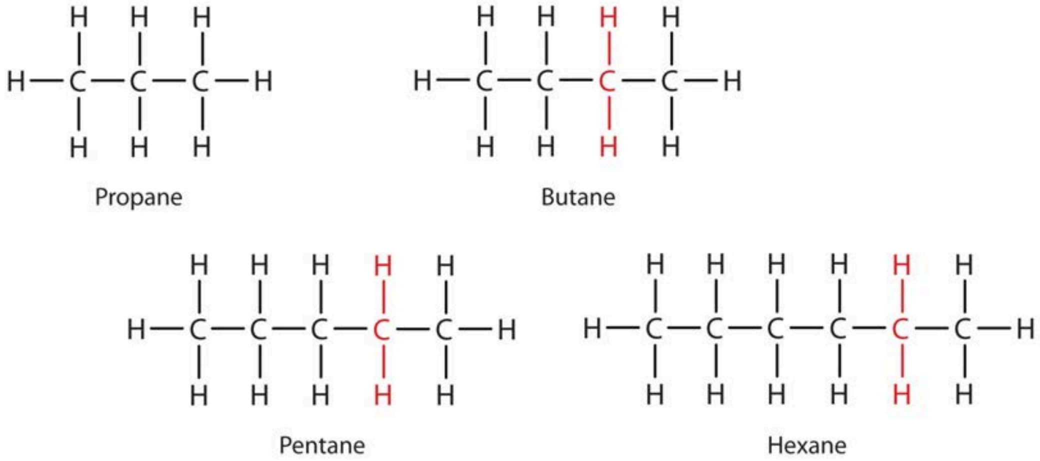


Figure 20.1f. Members of a Homologous Series. Each succeeding formula incorporates one carbon atom and two hydrogen atoms more than the previous formula(credit: *Intro Chemistry: GOB (V. 1.0).*, CC BY-NC-SA 4.0).

The principle of homology allows us to write a general formula for alkanes: C_nH_{2n+2}. Using this formula, we can write a molecular formula for any alkane with a given number of carbon atoms. For example, an alkane with eight carbon atoms has the molecular formula $C_8H_{(2 \times 8) + 2} = C_8H_{18}$.

The video What is Organic Chemistry below gives an introduction to alkanes.

Watch What Is Organic Chemistry?: Crash Course Organic Chemistry #1 – YouTube (10 min) (https://youtu.be/PmvLB5dIEp8?)

Physical Properties of Alkanes

Because alkanes have relatively predictable physical properties and undergo relatively few chemical reactions other than combustion, they serve as a basis of comparison for the properties of many other organic compound families. Let's consider their physical properties first.

Table 20.1b. describes some of the properties of some of the first 10 straight-chain alkanes. Because alkane molecules are nonpolar, they are insoluble in water, which is a polar solvent, but are soluble in nonpolar and slightly polar solvents. Consequently, alkanes themselves are commonly used as solvents for organic substances of low polarity, such as fats, oils, and waxes. Nearly all alkanes have densities less than 1.0 g/mL and are therefore less dense than water (the density of H_2O is 1.00 g/mL at 20°C). These properties explain why oil and grease do not mix with water but rather float on its surface as demonstrated in Figure 20.1g.

Table 20.1b. Physical Properties of Some Alkanes

Molecular Name	Formula	Melting Point (°C)	Boiling Point (°C)	Density (20°C)*	Physical State (at 20°C)
methane	CH_4	−182	−164	0.668 g/L	gas
ethane	C_2H_6	−183	−89	1.265 g/L	gas
propane	C_3H_8	−190	−42	1.867 g/L	gas
butane	C_4H_{10}	−138	−1	2.493 g/L	gas
pentane	C_5H_{12}	−130	36	0.626 g/mL	liquid
hexane	C_6H_{14}	−95	69	0.659 g/mL	liquid
octane	C_8H_{18}	−57	125	0.703 g/mL	liquid
decane	$C_{10}H_{22}$	−30	174	0.730 g/mL	liquid

***Note the change in units going from gases (grams per liter) to liquids (grams per milliliter). Gas densities are at 1 atm pressure.**

Table source: "12.6: Physical Properties of Alkanes" In *Basics of GOB Chemistry (Ball et al.)*, CC BY-NC-SA 4.0.

Table 20.1b. indicates that the first four members of the alkane series are gases at ordinary temperatures. Natural gas is composed chiefly of methane, which has a density of about 0.67 g/L. The density of air is about 1.29 g/L. Because natural gas is less dense than air, it rises. When a natural-gas leak is detected and shut off in a room, the gas can be removed by opening an upper window. On the other hand, bottled gas can be either propane (density 1.88 g/L) or butanes (a mixture of butane and isobutane; density about 2.5 g/L). Both are much heavier than air (density 1.2 g/L). If bottled gas escapes into a building, it collects near the floor. This presents a much more serious fire hazard than a natural-gas leak because it is more difficult to rid the room of the heavier gas.

Also shown in Table 20.1b are the boiling points of the straight-chain alkanes increase with increasing molar mass. This general rule holds true for the straight-chain homologs of all organic compound families. Larger molecules have greater surface areas and consequently interact more strongly; more energy is therefore required to separate them. For a given molar mass, the boiling points of alkanes are relatively low because these nonpolar molecules have only weak dispersion forces to hold them together in the liquid state.

Figure 20.1g. Oil Spills. Crude oil coats the water's surface in the Gulf of Mexico after the Deepwater Horizon oil rig sank following an explosion. The leak was a mile below the surface, making it difficult to estimate the size of the spill. One liter of oil can create a slick 2.5 hectares (6.3 acres) in size. This and similar spills provide a reminder that hydrocarbons and water don't mix. (Credit: *NASA Goddard / MODIS Rapid Response Team*, NASA terms of use).

Spotlight on Everyday Chemistry: Characteristics of Alkanes

Hydrocarbons are the simplest organic compounds, but they have interesting physiological effects. These effects depend on the size of the hydrocarbon molecules and where on or in the body they are applied. Alkanes of low molar mass—those with from 1 to approximately 10 or so carbon atoms—are gases or light liquids that act as anesthetics. Inhaling ("sniffing") these hydrocarbons in gasoline or aerosol propellants for their intoxicating effect is a major health problem that can lead to liver, kidney, or brain damage or to immediate death by asphyxiation by excluding oxygen.

Swallowed, liquid alkanes do little harm while in the stomach. In the lungs, however, they cause "chemical" pneumonia by dissolving fatlike molecules from cell membranes in the tiny air sacs (alveoli). The lungs become unable to expel fluids, just as in pneumonia caused by bacteria or viruses. People who swallow gasoline or other liquid alkane mixtures should not be made to vomit, as this would increase the chance of getting alkanes into the lungs. (There is no home-treatment antidote for gasoline poisoning; call a poison control center.)

Figure 20.1h. Butane is a hydrocarbon with the formula [latex]ce{C4H10}\) and is a gas at room temperature and atmospheric pressure. Under excess pressures, it can be liquidized like the fuel shown in this butane lighters. (Credit: work by Frank Vincentz, CC BY-SA 3.0)

Liquid alkanes with approximately 5–16 carbon atoms per molecule wash away natural skin oils and cause drying and chapping of the skin, while heavier liquid alkanes (those with approximately 17 or more carbon atoms per molecule) act as emollients (skin softeners). Such alkane mixtures as mineral oil and petroleum jelly can be applied as a protective film. Water and aqueous solutions such as urine will not dissolve such a film, which explains why petroleum jelly protects a baby's tender skin from diaper rash.

Attribution & References

Except where otherwise noted, this page is adapted by Adrienne Richards from:

- "12.0: Prelude to Organic Chemistry - Alkanes and Halogenated Hydrocarbons," "12.2: Structures and Names of Alkanes," "12.6: Physical Properties of Alkanes" and "12.7: Chemical Properties of Alkanes" In *Basics of General, Organic, and Biological Chemistry (Ball et al.)* by David W. Ball, John W. Hill, and Rhonda J. Scott (LibreTexts), licensed under CC BY-NC-SA 4.0. / A derivative of *Introduction to Chemistry: General, Organic, and Biological (V. 1.0),* CC BY-NC-SA 3.0. / Content from individual pages has been remixed into this one page. Tables and images are attributed individually.
- Except where otherwise noted, content from the 2nd paragraph under Alkanes heading through Figure 20.1 c is adapted from "1.6 sp3 Hybrid Orbitals and the Structure of Methane" In *Organic Chemistry (OpenStax)* by John McMurray, licensed under CC BY-NC-SA 4.0. Access for free at *Organic Chemistry (OpenStax)* (https://openstax.org/books/organic-chemistry/pages/1-why-this-chapter)
- Figure 20.1a is adapted from "1.4 Development of Chemical Bonding Theory" In *Organic Chemistry*

20.2 ALKANE FORMULAS

Learning Objectives

By the end of this section, you will be able to:

- Write molecular formulas for alkanes
- Draw structural formulas of the first 10 alkanes
- Write condensed structural formulas for alkanes given complete structural formulas.
- Draw line structures given condensed or structural formulas.

Types of Formulas to Represent Hydrocarbons

We use several kinds of formulas to describe organic compounds. A ***molecular formula*** shows only the kinds and numbers of atoms in a molecule. The general formula for alkanes: C_nH_{2n+2}. Using this formula, we can write a molecular formula for any alkane with a given number of carbon atoms. Table 20.2a. shows the molecular formulas of the first 10 straight-chain alkanes.

Table 20.2a. The First 10 Straight-Chain Alkane Molecular Formulas

Name	Molecular Formula (C_nH_{2n+2})
methane	CH_4
ethane	C_2H_6
propane	C_3H_8
butane	C_4H_{10}
pentane	C_5H_{12}
hexane	C_6H_{14}
heptane	C_7H_{16}
octane	C_8H_{18}
nonane	C_9H_{20}
decane	$C_{10}H_{22}$

Table source: "12.2: Structures and Names of Alkanes" In *Basics of GOB Chemistry (Ball et al.)*, CC BY-NC-SA 4.0.

For example in Table 20.2a. above, the molecular formula C_4H_{10} tells us there are 4 carbon atoms and 10 hydrogen atoms in a molecule, but it doesn't distinguish between butane and isobutane. A structural formula shows all the carbon and hydrogen atoms and the bonds attaching them. Thus, structural formulas identify the specific isomers (learned in the next section) by showing the order of attachment of the various atoms.

Unfortunately, **structural formulas** are difficult to type/write and take up a lot of space. Chemists often use condensed structural formulas to alleviate these problems. The condensed structural formulas for the first 10 alkanes are demonstrated in Table 20.2a. Parentheses in condensed structural formulas indicate that the enclosed grouping of atoms is attached to the adjacent carbon atom. The condensed formulas show hydrogen atoms right next to the carbon atoms to which they are attached, as illustrated in Figure 20.2a. for butane:

Figure 20.2a. Structural and condensed formula for butane (credit: *Intro Chem:GOB (V. 1.0)*, CC BY-NC-SA 4.0.)

The ultimate condensed formula is a **line structure formula**. In this type of structure, carbon atoms are not symbolized with a C, but represented by each end of a line or bend in a line. Hydrogen atoms are not drawn if they are attached to a carbon. Other atoms besides carbon and hydrogen are represented by their elemental symbols. For example in Figure 20.2b., we can represent pentane ($CH_3CH_2CH_2CH_2CH_3$) and isopentane [$(CH_3)_2CHCH_2CH_3$] as follows:

Figure 20.2b. Line structure for pentane and isopentane (credit: *Intro Chem:GOB (V. 1.0)*, CC BY-NC-SA 4.0.)

Drawing organic molecules can be challenging. There is software available to assist with drawing molecules. Refer to Appendix B: Organic Chemistry Software for more details and tutorials.

In summary, the following Figure 20.2c. demonstrates the structural (expanded), condensed and line structure formulas.

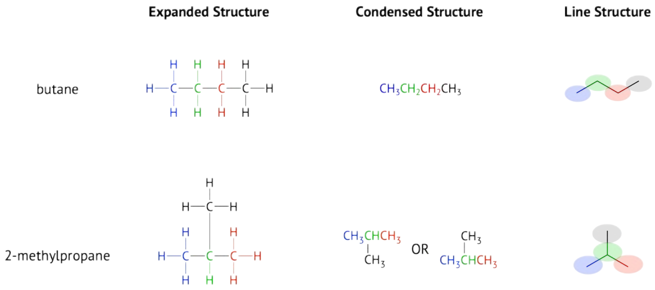
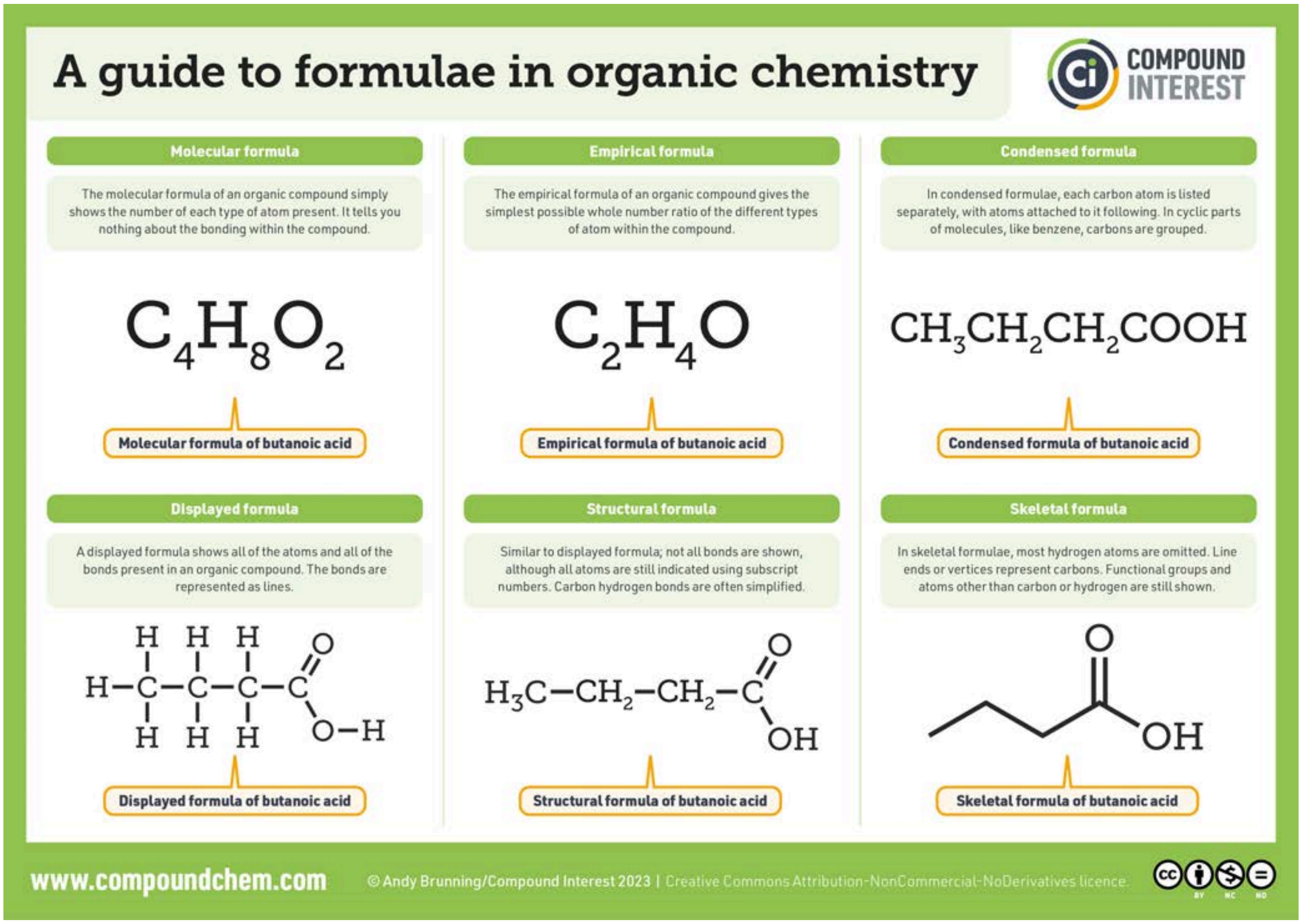


Figure 20.2c. Structural representations for butane and its isomer, 2-methylpropane. (The colours are used to help identify carbons and do not represent any special properties.) (credit: *Fundamentals of GOB (McMurry et al.),* CC BY-NC-SA 3.0)

For a summary chart of the formulae used in organic chemistry, infographic 20.2a. demonstrates the different ways to represent organic compounds. Molecular and empirical formulas are explained as the simplest followed by condensed, structural and skeletal (or line) formulae.



A guide to formulae in organic chemistry

COMPOUND INTEREST

Molecular formula

The molecular formula of an organic compound simply shows the number of each type of atom present. It tells you nothing about the bonding within the compound.

$C_4H_8O_2$

Molecular formula of butanoic acid

Empirical formula

The empirical formula of an organic compound gives the simplest possible whole number ratio of the different types of atom within the compound.

C_2H_4O

Empirical formula of butanoic acid

Condensed formula

In condensed formulae, each carbon atom is listed separately, with atoms attached to it following. In cyclic parts of molecules, like benzene, carbons are grouped.

$CH_3CH_2CH_2COOH$

Condensed formula of butanoic acid

Displayed formula

A displayed formula shows all of the atoms and all of the bonds present in an organic compound. The bonds are represented as lines.

Displayed formula of butanoic acid

Structural formula

Similar to displayed formula; not all bonds are shown, although all atoms are still indicated using subscript numbers. Carbon hydrogen bonds are often simplified.

Structural formula of butanoic acid

Skeletal formula

In skeletal formulae, most hydrogen atoms are omitted. Line ends or vertices represent carbons. Functional groups and atoms other than carbon or hydrogen are still shown.

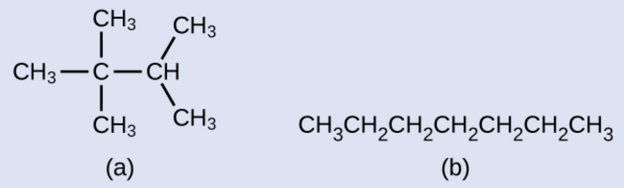
Skeletal formula of butanoic acid

www.compoundchem.com

Infographic 20.2a. Read more about "A Brief Guide to Types of Organic Chemistry Formulae (https://www.compoundchem.com/2014/04/11/a-brief-guide-to-types-of-organic-chemistry-formula/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary of infographic 20.2a [New tab].

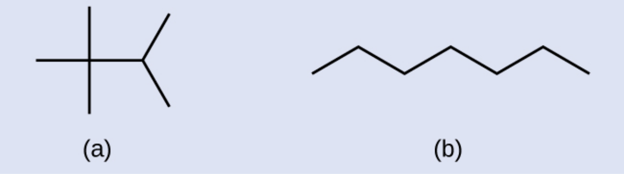
Example 20.2a

Draw the line structures for these two molecules:



Solution

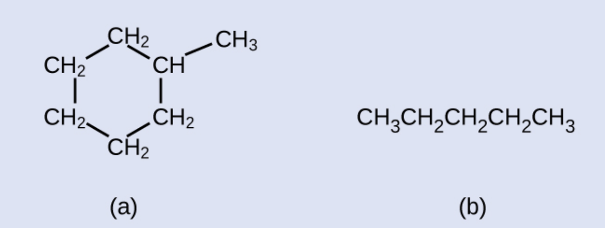
Each carbon atom is converted into the end of a line or the place where lines intersect. All hydrogen atoms attached to the carbon atoms are left out of the structure (although we still need to recognize they are there):



Example & image source: *General Chemistry 1 & 2* , CC BY 4.0.

Exercise 20.2a

Draw the line structures for these two molecules:

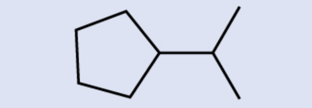


Check your answer[1]

Example & image source: *General Chemistry 1 & 2* , CC BY 4.0.

Example 20.2b

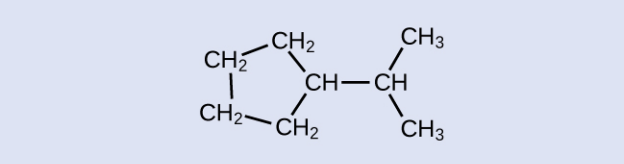
Identify the molecular formula of the molecule represented here:



Solution

There are eight places where lines intersect or end, meaning that there are eight carbon atoms in the molecule. Since we know that carbon atoms tend to make four bonds, each carbon atom will have the number of hydrogen atoms that are required for four bonds. This compound contains 16 hydrogen atoms for a molecular formula of C_8H_{16}.

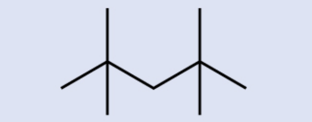
Location of the hydrogen atoms:



Example & image source: *General Chemistry 1 & 2* , CC BY 4.0.

Exercise 20.2b

Identify the molecular formula of the molecule represented here:



Check your Answer[2]

Example & image source: *General Chemistry 1 & 2* , CC BY 4.0.

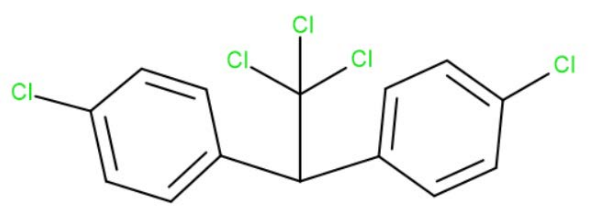
Exercise 20.2c

Identifying carbons in a structure

By looking at the chemical structure of DDT (Dichlorodiphenyltrichloroethane), click on the location of each carbon within the DDT structure.

Exercise 20.2c (Text version)

Identify the location of each carbon atom in the DDT structure. DDT is dichlorodiphenyltrichloroethane. It contains two aromatic rings connected by one carbon of an ethane structure. The molecular formula is $C_{14}H_9Cl_5$. (Structure is shown in as a line structure.)



Check Your Answer:[3]

Activity source: "Identifying carbons in line structure" by Samantha Sullivan Sauer, licensed under CC BY-NC 4.0

Links to Enhanced Learning

- For an interactive practice link to the interactive activity on Hydrocarbons [New tab] (https://h5pstudio.ecampusontario.ca/content/18383) to determine the number of hydrogens in an organic compound from Jessica Anderson.

Attribution & References

Except where otherwise noted, this page is adapted by Adrienne Richards from

- "12.2: Structures and Names of Alkanes", "12.4: Condensed Structural and Line-Angle Formulas" In *Basics of General, Organic, and Biological Chemistry (Ball et al.)* by David W. Ball, John W. Hill, and Rhonda J. Scott via LibreTexts, licensed under CC BY-NC-SA 4.0. / A derivative of *Introduction to Chemistry: GOB (v. 1.0),* CC BY-NC 3.0
- Individual pages have been remixed into this version, including
    - Examples 1 & 2 are adapted from "18.1 Hydrocarbons (https://boisestate.pressbooks.pub/chemistry/chapter/21-1-hydrocarbons/)" In *General Chemistry 1 & 2* by Rice University, a derivative of *Chemistry (Open Stax)* by Paul Flowers, Klaus Theopold, Richard Langley & William

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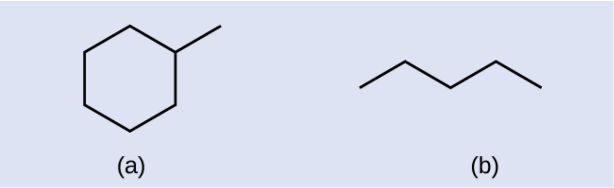
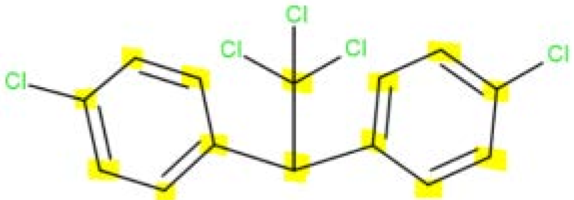
- “12.4: Drawing Organic Structures” by Lisa Sharpe Elles, In *Map: Fundamentals of General Organic and Biological Chemistry (McMurry et al.),* CC BY-NC-SA 3.0. / A derivative of *Basics of GOB (Ball et al.),* CC BY-NC-SA 4.0. which is a LibreTexts version of *Introduction to Chemistry: GOB (v. 1.0),* CC BY-NC 3.0

Notes

1. 

2. C_9H_{20}
3. Carbons are highlighted in yellow in this image. 

There are 14 carbon atoms. Six in each aromatic ring, one that connects the rings together and one that branches off the middle carbon.

20.3 ISOMERS OF ALKANES AND IUPAC NOMENCLATURE

Learning Objectives

By the end of this section, you will be able to:

- Identify simple alkanes as straight-chain or branched-chain.
- Describe and recognize structural and functional group isomers.
- Name alkanes by the IUPAC system and write formulas for alkanes given IUPAC names

Isomers

Hydrocarbons with the same formula, including alkanes, can have different structures. For example, two alkanes have the formula C_4H_{10}: They are called *n*-butane and 2-methylpropane (or isobutane), and have the following structural formulas as shown in Figure 20.3a:

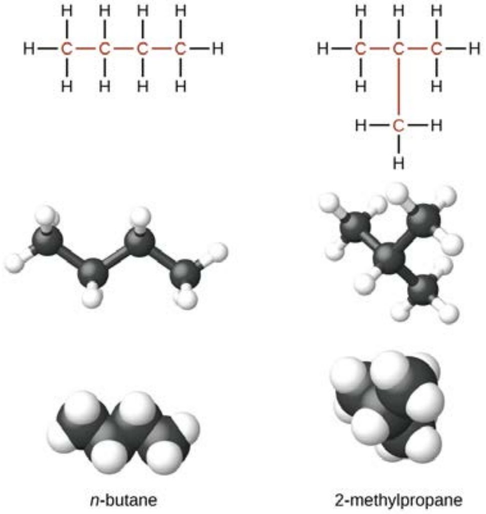


Figure 20.3a. Structural and ball-and-stick formulas for butane and 2-methylpropane (credit: *General Chemistry 1 & 2* , CC BY 4.0).

The compounds *n*-butane and 2-methylpropane are structural isomers (the term constitutional isomers is also commonly used). Constitutional **isomers** have the same molecular formula but different spatial arrangements of the atoms in their molecules. The *n*-butane molecule contains an *unbranched chain*, meaning that no carbon atom is bonded to more than two other carbon atoms. We use the term *normal*, or the prefix *n*, to refer to a chain of carbon atoms without branching. The compound 2–methylpropane has a branched chain (the carbon atom in the center of the structural formula is bonded to three other carbon atoms).

Recall from section 20.2, Table 20.3a. which shows the molecular formula and condensed structural formulas for the first 10 straight-chain alkanes. Table 20.3a also shows the number of isomers for each alkane. The number of isomers increases rapidly as the number of carbon atoms increases.

Table 20.3a. The First 10 Straight-Chain Alkane Formulas and Isomers

Name	Molecular Formula (C_nH_{2n+2})	Condensed Structural Formula	Number of Possible Isomers
methane	CH_4	CH_4	—
ethane	C_2H_6	CH_3CH_3	—
propane	C_3H_8	$CH_3CH_2CH_3$	—
butane	C_4H_{10}	$CH_3CH_2CH_2CH_3$	2
pentane	C_5H_{12}	$CH_3CH_2CH_2CH_2CH_3$	3
hexane	C_6H_{14}	$CH_3CH_2CH_2CH_2CH_2CH_3$	5
heptane	C_7H_{16}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$	9
octane	C_8H_{18}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	18
nonane	C_9H_{20}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	35
decane	$C_{10}H_{22}$	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	75

Table source: "12.2: Structures and Names of Alkanes" In *Basics of GOB Chemistry (Ball et al.)*, CC BY-NC-SA 4.0.

Identifying isomers from structural formulae is not as easy as it looks. Structural formulae that look different may actually represent the same isomers. For example, the three structures in Figure 20.3b all represent the same molecule, *n*-butane, and hence are not different isomers. They are identical because each contains an unbranched chain of four carbon atoms.

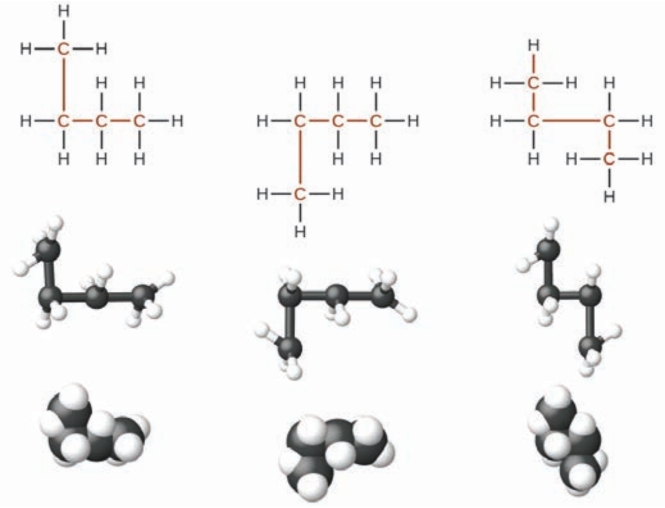


Figure 20.3b. These three representations of the structure of n-butane are not isomers because they all contain the same arrangement of atoms and bonds (credit: *General Chemistry 1 & 2* , CC BY 4.0.)

When identifying isomers, it is useful to trace the carbon backbone with your finger or a pencil and count carbons until you need to lift your hand or pencil to get the another carbon. Try this with each of the above arrangements of four carbons above in Figure 20.3b. Butane has a continuous chain of four carbons no matter how the bonds are rotated – you can connect the carbons in a line without lifting your finger from the page. In a later portion of this chapter, you will learn how to systematically name compounds by counting the number of carbons in the longest continuous chain and identifying any functional groups present.

Adding one more carbon to the butane chain gives pentane, which has the formula, C_5H_{12}. Pentane and its two branched-chain isomers are shown below in Figure 20.3c. The compound at the far left is pentane because it has all five carbon atoms in a continuous chain. The compound in the middle is isopentane; like isobutane, it has a one CH_3 branch off the second carbon atom of the continuous chain. The compound at the far right, discovered after the other two, was named neopentane (from the Greek *neos*, meaning “new”). Although all three have the same molecular formula, they have different properties, including boiling points: pentane, 36.1°C; isopentane, 27.7°C; and neopentane, 9.5°C. The names isopentane and neopentane are common names for these molecules. As mentioned above, we will learn the systematic rules for naming compounds next.

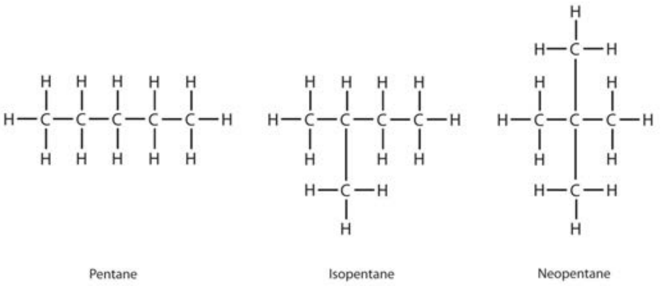
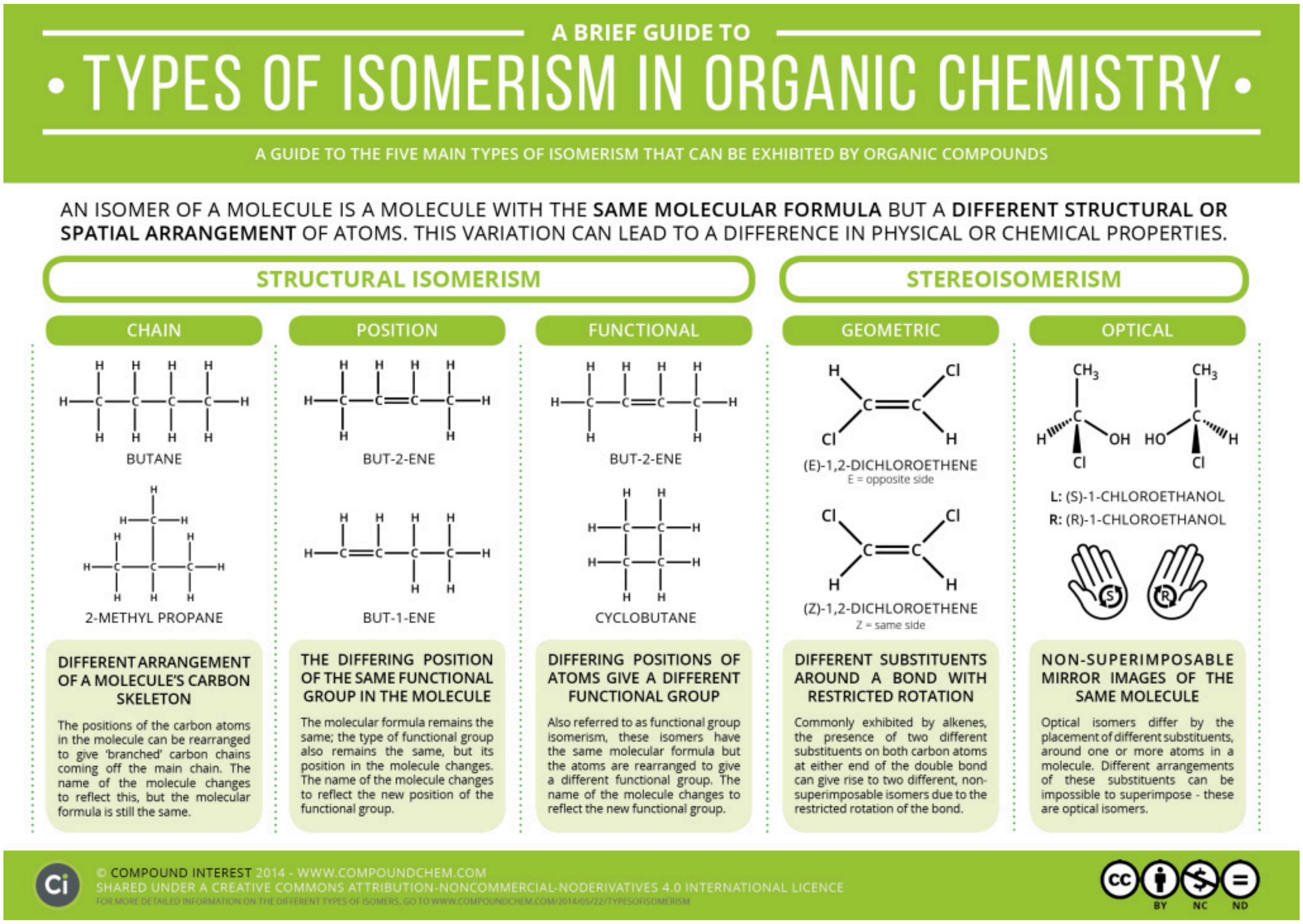


Figure 20.3c. Structural formulas representing 3 isomers of pentane. (Credit: *Introduction to Chemistry: GOB (V. 1.0).* ,CC BY-NC-SA 3.0.)

A summary of isomers is illustrated in infographic 20.3a, which includes structural isomerism and stereoisomerism.



A BRIEF GUIDE TO

• TYPES OF ISOMERISM IN ORGANIC CHEMISTRY •

A GUIDE TO THE FIVE MAIN TYPES OF ISOMERISM THAT CAN BE EXHIBITED BY ORGANIC COMPOUNDS

AN ISOMER OF A MOLECULE IS A MOLECULE WITH THE **SAME MOLECULAR FORMULA** BUT A **DIFFERENT STRUCTURAL OR SPATIAL ARRANGEMENT** OF ATOMS. THIS VARIATION CAN LEAD TO A DIFFERENCE IN PHYSICAL OR CHEMICAL PROPERTIES.

STRUCTURAL ISOMERISM

CHAIN

BUTANE

2-METHYL PROPANE

DIFFERENT ARRANGEMENT OF A MOLECULE'S CARBON SKELETON

The positions of the carbon atoms in the molecule can be rearranged to give 'branched' carbon chains coming off the main chain. The name of the molecule changes to reflect this, but the molecular formula is still the same.

POSITION

BUT-2-ENE

BUT-1-ENE

THE DIFFERING POSITION OF THE SAME FUNCTIONAL GROUP IN THE MOLECULE

The molecular formula remains the same; the type of functional group also remains the same, but its position in the molecule changes. The name of the molecule changes to reflect the new position of the functional group.

FUNCTIONAL

BUT-2-ENE

CYCLOBUTANE

DIFFERING POSITIONS OF ATOMS GIVE A DIFFERENT FUNCTIONAL GROUP

Also referred to as functional group isomerism, these isomers have the same molecular formula but the atoms are rearranged to give a different functional group. The name of the molecule changes to reflect the new functional group.

STEREOISOMERISM

GEOMETRIC

(E)-1,2-DICHLOROETHENE
E = opposite side

(Z)-1,2-DICHLOROETHENE
Z = same side

DIFFERENT SUBSTITUENTS AROUND A BOND WITH RESTRICTED ROTATION

Commonly exhibited by alkenes, the presence of two different substituents on both carbon atoms at either end of the double bond can give rise to two different, non-superimposable isomers due to the restricted rotation of the bond.

OPTICAL

L: (S)-1-CHLOROETHANOL
R: (R)-1-CHLOROETHANOL

NON-SUPERIMPOSABLE MIRROR IMAGES OF THE SAME MOLECULE

Optical isomers differ by the placement of different substituents, around one or more atoms in a molecule. Different arrangements of these substituents can be impossible to superimpose - these are optical isomers.

Infographic 20.3a. Read more about "A Brief Guide to Types of Isomerism in Organic Chemistry (https://www.compoundchem.com/2014/05/22/typesofisomerism/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary of infographic 20.3a [New tab].

IUPAC System of Nomenclature for Alkanes

Looking at Table 20.3a., there are 3 pentanes, 5 hexanes, 9 heptanes, and 18 octanes. It would be difficult to assign unique individual names that we could remember. A systematic way of naming hydrocarbons and other organic compounds has been devised by the International Union of Pure and Applied Chemistry (IUPAC). These rules, used worldwide, are known as the IUPAC System of Nomenclature. A stem name (Table 20.3b.) indicates the number of carbon atoms in the longest continuous chain (LCC). Atoms or groups attached to this carbon chain, called *substituents*, are then named, with their positions indicated by numbers. For now, we will consider only those substituents called alkyl groups.

Table 20.3b. Stems That Indicate the Number of Carbon Atoms in Organic Molecules

Stem	Number
meth-	1
eth-	2
prop-	3
but-	4
pent-	5
hex-	6
hept-	7
oct-	8
non-	9
dec-	10

Table source: “12.5: IUPAC Nomenclature” In *Basics of GOB Chemistry (Ball et al.)*, CC BY-NC-SA 4.0.

An alkyl group is a group of atoms that results when one hydrogen atom is removed from an alkane. The group is named by replacing the *-ane* suffix of the parent hydrocarbon with *-yl*. For example, the -CH_3 group derived from methane (CH_4) results from subtracting one hydrogen atom and is called a *methyl group*. The alkyl groups we will use most frequently are listed in Table 20.3c. Alkyl groups are not independent molecules; they are parts of molecules that we consider as a unit to name compounds systematically.

Table 20.3c. Common Alkyl Groups

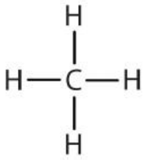
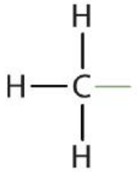
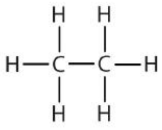
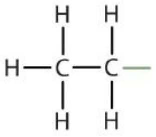
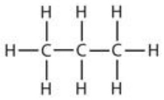
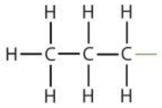
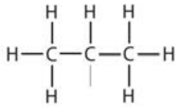
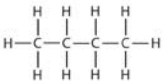
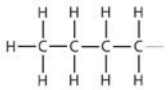
Parent Alkane		Alkyl Group		Condensed Structural Formula
methane		methyl		CH_3-
ethane		ethyl		CH_3CH_2-
propane		propyl		$CH_3CH_2CH_2-$
		isopropyl		$(CH_3)_2CH-$
butane		butyl*		$CH_3CH_2CH_2CH_2-$

Table 20.3c. note: *There are four butyl groups, two derived from butane and two from isobutane. We will introduce the other three where appropriate. (Image credits: *Introduction to Chemistry: GOB (V. 1.0).* , CC BY-NC-SA 3.0).

Simplified IUPAC rules for naming alkanes are as follows (demonstrated in Example 20.3a.).

1. **Name alkanes according to the LCC (longest continuous chain) of carbon atoms in the molecule (rather than the total number of carbon atoms).** This LCC, considered the parent chain, determines the base name, to which we add the suffix *–ane* to indicate that the molecule is an alkane.
2. **If the hydrocarbon is branched, number the carbon atoms of the LCC.** Numbers are assigned in the direction that gives the lowest numbers to the carbon atoms with attached substituents. Hyphens are used to separate numbers from the names of substituents; commas separate numbers from each other. (The LCC need not be written in a straight line; for example, the LCC in the following has five carbon atoms.)

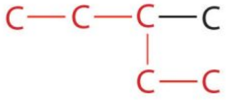


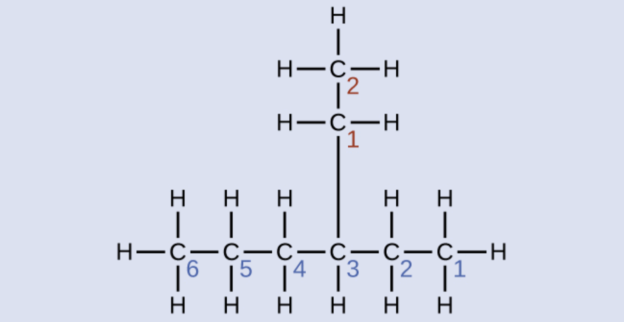
Figure 20.3d. An example showing that finding the longest carbon chain does not have to be in a straight line. (Credit: *Introduction to Chemistry: GOB (V. 1.0).* ,CC BY-NC-SA 3.0.)

3. **Place the names of the substituent groups in alphabetical order before the name of the parent compound.** If the same alkyl group appears more than once, the numbers of all the carbon atoms to which it is attached are expressed. If the same group appears more than once on the same carbon atom, the number of that carbon atom is repeated as many times as the group appears. Moreover, the number of identical groups is indicated by the Greek prefixes *di-*, *tri-*, *tetra-*, and so on. These prefixes are *not* considered in determining the alphabetical order of the substituents. For example, ethyl is listed before dimethyl; the di- is simply ignored. The last alkyl group named is prefixed to the name of the parent alkane to form one word.

When these rules are followed, every unique compound receives its own exclusive name. The rules enable us to not only name a compound from a given structure but also draw a structure from a given name. The best way to learn how to use the IUPAC system is to put it to work, not just memorize the rules. It's easier than it looks.

Example 20.3a

Name the molecule whose structure is shown here:



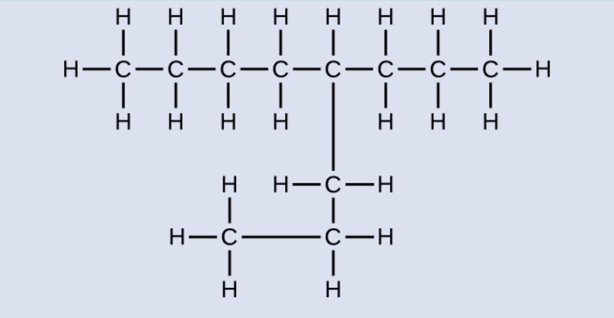
Solution

The longest carbon chain runs horizontally across the page and contains six carbon atoms (this makes the base of the name hexane, but we will also need to incorporate the name of the branch). In this case, we want to number from right to left (as shown by the blue numbers) so the branch is connected to carbon 3 (imagine the numbers from left to right—this would put the branch on carbon 4, violating our rules). The branch attached to position 3 of our chain contains two carbon atoms (numbered in red)—so we take our name for two carbons *eth-* and attach *-yl* at the end to signify we are describing a branch. Putting all the pieces together, this molecule is 3-ethylhexane.

Example & image source: *General Chemistry 1 & 2* , CC BY 4.0.

Exercise 20.3a

Name the following molecule:



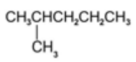
Check Your Answer[1]

Exercise & image source: *General Chemistry 1 & 2* , CC BY 4.0.

Example 20.3b

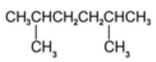
Name each compound:

1.



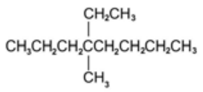
$CH_3\underset{CH_3}{\underset{|}{C}}HCH_2CH_2CH_3$

2.



$CH_3\underset{CH_3}{\underset{|}{C}}HCH_2CH_2\underset{CH_3}{\underset{|}{C}}HCH_3$

3.



$CH_3CH_2CH_2\overset{CH_2CH_3}{\overset{|}{\underset{CH_3}{\underset{|}{C}}}}CH_2CH_2CH_2CH_3$

Solution

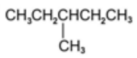
1. The LCC has five carbon atoms, and so the parent compound is pentane (rule 1). There is a methyl group (rule 2) attached to the second carbon atom of the pentane chain. The name is therefore 2-methylpentane.
2. The LCC has six carbon atoms, so the parent compound is hexane (rule 1). Methyl groups (rule 2) are attached to the second and fifth carbon atoms. The name is 2,5-dimethylhexane.
3. The LCC has eight carbon atoms, so the parent compound is octane (rule 1). There are methyl and ethyl groups (rule 2), both attached to the fourth carbon atom (counting from the *right* gives this carbon atom a lower number; rule 3). The correct name is thus 4-ethyl-4-methyloctane.

Example & image source: *Introduction to Chemistry: GOB (V. 1.0).*, CC BY-NC-SA 3.0

Exercise 20.3b

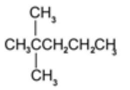
Name each compound.

1.



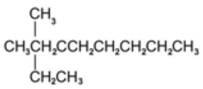
$CH_3CH_2\underset{CH_3}{\underset{|}{C}}HCH_2CH_3$

2.



$CH_3\overset{CH_3}{\overset{|}{\underset{CH_3}{\underset{|}{C}}}}CH_2CH_2CH_3$

3.



$CH_3\overset{CH_3}{\overset{|}{\underset{CH_2CH_3}{\underset{|}{C}}}}H_2CCH_2CH_2CH_2CH_2CH_3$

Check your answer[2]

Exercise & image source: *Introduction to Chemistry: GOB (V. 1.0).*, CC BY-NC-SA 3.0

Example 20.3c

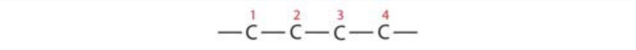
Draw the structure for each compound.

a. 2,3-dimethylbutane
b. 4-ethyl-2-methylheptane

Solution

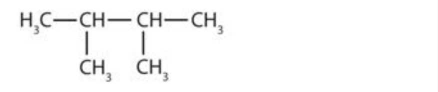
In drawing structures, always start with the parent chain.

The parent chain is butane, indicating four carbon atoms in the LCC.



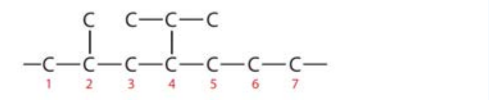
Then add the groups at their proper positions. You can number the parent chain from either direction as long as you are consistent; just don't change directions before the structure is done. The name indicates two methyl (CH_3) groups, one on the second carbon atom and one on the third.

Finally, fill in all the hydrogen atoms, keeping in mind that each carbon atom must have four bonds.

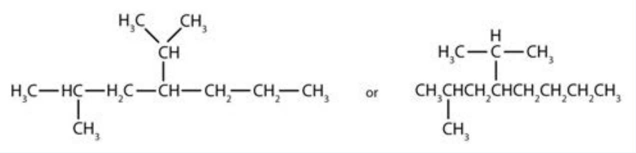


The parent chain is heptane in this case, indicating seven carbon atoms in the LCC. –C–C–C–C–C–C–C–

Adding the groups at their proper positions gives



Filling in all the hydrogen atoms gives the following condensed structural formulas:



Note that the bonds (dashes) can be shown or not; sometimes they are needed for spacing.

Example & image source: *Introduction to Chemistry: GOB (V. 1.0).*, CC BY-NC-SA 3.0

Exercise 20.3c

Draw the structure for each compound.

4-ethyloctane

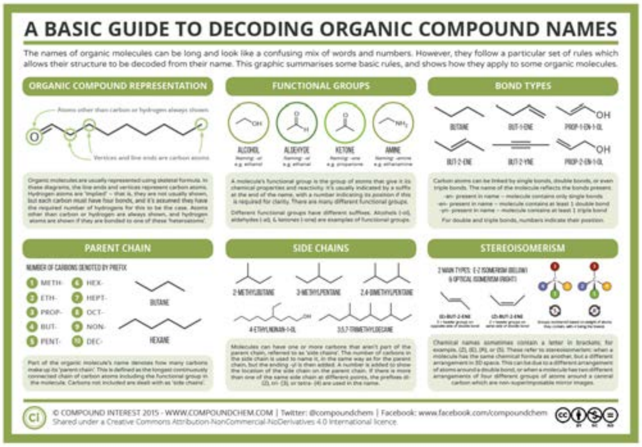
a. 3-ethyl-2-methylpentane
b. 3,3,5-trimethylheptane

Check your answer [3]

Want more practice naming alkanes?

Watch the video tutorial Naming simple alkanes (10 mins) on YouTube (https://youtu.be/NRFPvLp3r3g) to review the nomenclature process.

For a summary on naming organic compounds, infographic 20.3b looks at the rules for decoding the types of organic compounds and how to name them.



A BASIC GUIDE TO DECODING ORGANIC COMPOUND NAMES

The names of organic molecules can be long and look like a confusing mix of words and numbers. However, they follow a particular set of rules which allows their structure to be decoded from their name. This graphic summarises some basic rules, and shows how they apply to some organic molecules.

ORGANIC COMPOUND REPRESENTATION

FUNCTIONAL GROUPS

BOND TYPES

PARENT CHAIN

SIDE CHAINS

STEREOISOMERISM

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Infographic 20.3b. Read more about "A Basic Guide to Decoding Organic Compound Names (https://www.compoundchem.com/2015/08/27/org-comp-names/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary [New tab].

Links to Enhanced Learning

For a general introduction to organic chemistry naming beyond the basic alkane naming, watch The Basics of Organic Nomenclature: Crash Course Organic Chemistry #2 – YouTube. (https://www.youtube.com/watch?v=HhT2E7wuAgg&list=PL8dPuuaLjXtONguuhLdVmq0HTKS0jksS4&index=3)

For interactive practice questions on isomers link to Organic Chemistry Practice (https://h5pstudio.ecampusontario.ca/content/18386) from eCampusOntario H5P Studio.

Attribution & References

Except where otherwise noted, this page is adapted by Adrienne Richards from the following sources

- "12.3: The Structure of Organic Molecules – Alkanes and Their Isomers" & "12.6: Naming Alkanes" In *Map: Fundamentals of General Organic and Biological Chemistry (McMurry et al.)* by LibreTexts, licensed under CC BY-NC-SA 3.0 . / A derivative of 12.5: IUPAC Nomenclature, 12.2: Structures and Names of Alkanes, & 12.3: Branched-Chain Alkanes In *Basics of GOB (Ball et al.),* CC BY-NC-SA 4.0 a LibreTexts version of *Introduction to Chemistry: GOB (v. 1.0),* CC BY-NC 3.0
- "18.1 Hydrocarbons (https://boisestate.pressbooks.pub/chemistry/chapter/21-1-hydrocarbons/)" In *General Chemistry 1 & 2* by Rice University, a derivative of *Chemistry (Open Stax)* by Paul Flowers, Klaus Theopold, Richard Langley & William R. Robinson and is licensed under CC BY 4.0. Access for free at *Chemistry (OpenStax) (https://openstax.org/books/chemistry/pages/1-introduction)*
- "12.2: Structures and Names of Alkanes" In *Basics of General, Organic, and Biological Chemistry (Ball et al.)* by David W. Ball, John W. Hill, and Rhonda J. Scott via LibreTexts, licensed under CC BY-NC-SA 4.0. / A derivative of *Introduction to Chemistry: General, Organic, and Biological (V. 1.0),* CC BY-NC-SA 3.0.

Notes

1. 4-propyloctane
2.
   1. 3-methylpentane
   2. 2, 2-dimethylpentane

3. 2-ethyl 2-methyloctane

3\.

a. See the image: 4-Ethyloctane | C10H22 | CID 85925 - PubChem (nih.gov)
b. See the image: 3-Ethyl-2-methylpentane | C8H18 | CID 11863 - PubChem (nih.gov)
c. See the image: 3,3,5-Trimethylheptane | C10H22 | CID 23544 - PubChem (nih.gov)

20.4 CYCLOALKANES

Learning Objectives

By the end of this section, you will be able to:

- Name cycloalkanes given their formulas and write formulas for these compounds given their names.

Cylcoalkanes

The hydrocarbons we have encountered so far have been composed of molecules with open-ended chains of carbon atoms. When a chain contains three or more carbon atoms, the atoms can join to form *ring* or *cyclic* structures. The simplest of these cyclic hydrocarbons has the formula C_3H_6. Each carbon atom has two hydrogen atoms attached (Figure 20.4a.) and is called cyclopropane.

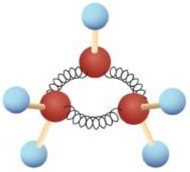


Figure 20.4a. Ball-and-Spring Model of Cyclopropane. The springs are bent to join the carbon atoms. (Credit: *Intro Chem: GOB (V. 1.0).* ,*CC BY-NC-SA 3.0*)

Spotlight on Everyday Chemistry: Cyclopropane (C_3H_6) as an Anesthetic

With its boiling point of −33°C, cyclopropane is a gas at room temperature. It is also a potent, quick-acting anesthetic with few undesirable side effects in the body. It is no longer used in surgery, however, because it forms explosive mixtures with air at nearly all concentrations. A line structure of cyclopropane is shown in Figure 20.4b.

The cycloalkanes—cyclic hydrocarbons with only single bonds—are named by adding the prefix *cyclo-* to the name of the open-chain compound having the same number of carbon atoms as there are in the ring. Thus the name for the cyclic compound C_4H_8 is cyclobutane. The carbon atoms in cyclic compounds can be represented by *line structure formulas* that result in regular geometric figures. Keep in mind, however, that each corner of the geometric figure represents a carbon atom plus as many hydrogen atoms as needed to give each carbon atom four bonds. Figure 20.4 demonstrates the line structure formulas of both cyclopropane and cyclohexane.

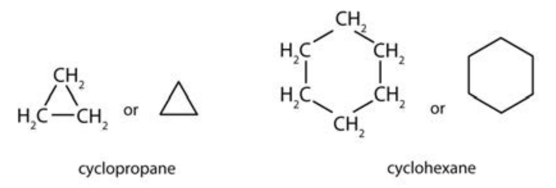


Figure 20.4b. The line structure and geometric shapes of cyclopropane and cyclohexane. (Credit: *Intro Chem: GOB (V. 1.0)*. ,CC BY-NC-SA 3.0.)

Some cyclic compounds have substituent groups attached. Example 20.4a interprets the name of a cycloalkane with a single substituent group.

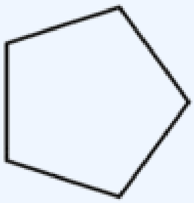
Example 20.4a

Draw the structure for each compound.

a. cyclopentane
b. methylcyclobutane

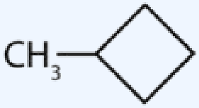
Solution

a. The name *cyclopentane* indicates a cyclic (cyclo) alkane with five (pent-) carbon atoms. It can be represented as a pentagon.



(Credit: *Intro Chem: GOB (V. 1.0).* ,*CC BY-NC-SA 3.0.*)

- The name *methylcyclobutane* indicates a cyclic alkane with four (but-) carbon atoms in the cyclic part. It can be represented as a square with a CH_3 group attached.



(Credit: *Intro Chem: GOB (V. 1.0).* ,CC BY-NC-SA 3.0.)

Exercise 20.4a

Draw the structure for each compound.

a. cycloheptane
b. ethylcyclohexane

Check Your Answer[1]

The properties of cyclic hydrocarbons are generally quite similar to those of the corresponding open-chain compounds. So cycloalkanes (with the exception of cyclopropane, which has a highly strained ring) act very much like noncyclic alkanes. Cyclic structures containing five or six carbon atoms, such as cyclopentane and cyclohexane, are particularly stable. We will see later that some carbohydrates (sugars) form five- or six-membered rings in solution.

The cyclopropane ring is strained because the C–C–C angles are 60°, and the preferred (tetrahedral) bond angle is 109.5°. (This strain is readily evident when you try to build a ball-and-stick model of cyclopropane; see Figure 20.4a.) Cyclopentane and cyclohexane rings have little strain because the C–C–C angles are near the preferred angles. Cyclohexane is shown in Figure 20.4b.

Substituted Cycloalkanes

We'll see numerous instances in future chapters where the chemistry of a given functional group is affected by being in a ring rather than an open chain. Because cyclic molecules are encountered in most pharmaceuticals and in all classes of biomolecules, including proteins, lipids, carbohydrates, and nucleic acids, it's important to understand the behaviour of cyclic structures.

Although we've only discussed open-chain compounds up to now, most organic compounds contain *rings* of carbon atoms. Chrysanthemic acid in Figure 20.4c, for instance, whose esters occur naturally as the active insecticidal constituents of chrysanthemum flowers, contains a three-membered (cyclopropane) ring.

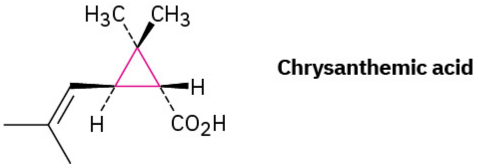


Figure 20.4c. The chemical structure shown is Chrysanthemic acid which shows a substituted cyclopropane (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0).

Prostaglandins, potent hormones that control an extraordinary variety of physiological functions in humans, contain a five-membered (cyclopentane) ring. An example of a prostaglandin is in Figure 20.4d.

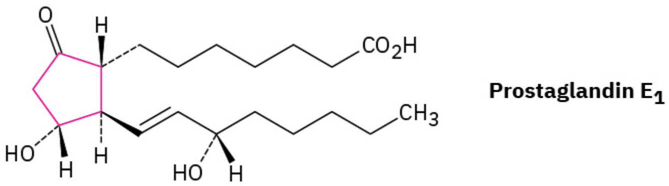
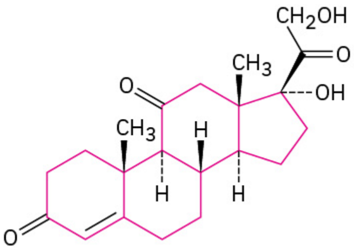


Figure 20.4d. The chemical structure shown is Prostaglandin E_1 which shows a substituted cyclopentane (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0).

Steroids, such as cortisone, contain four rings joined together—three six-membered (cyclohexane) and one five-membered.

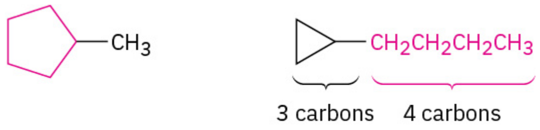


Cortisone

Figure 20.4e. The chemical structure shown is Cortisone which shows four substituted rings joined together. There are three cyclohexanes and one cyclopentane (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0).

Substituted cycloalkanes are named by rules similar to those we saw for open-chain alkanes. For most compounds, there are only two steps.

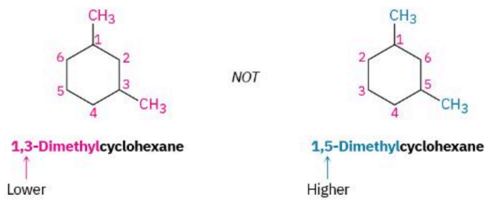
1. Find the parent. Count the number of carbon atoms in the ring and the number in the largest substituent. If the number of carbon atoms in the ring is equal to or greater than the number in the substituent, the compound is named as an alkyl-substituted cycloalkane. If the number of carbon atoms in the largest substituent is greater than the number in the ring, the compound is named as a cycloalkyl-substituted alkane. Refer to Figure 20.4f. for examples of substituted cycloalkanes.



Methylcyclopentane **1-Cyclopropylbutane**

Figure 20.4f. Alkyl substituted cycloalkanes methylcyclopentane and 1-cyclopropyl butane. (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0)

2. Number the substituents and write the name. For an alkyl- or halo-substituted cycloalkane, choose a point of attachment as carbon 1 and number the substituents on the ring so that the *second* substituent has as low a number as possible. If ambiguity still exists, number so that the third or fourth substituent has as low a number as possible, until a point of difference is found as shown in the example within Figure 20.4g.



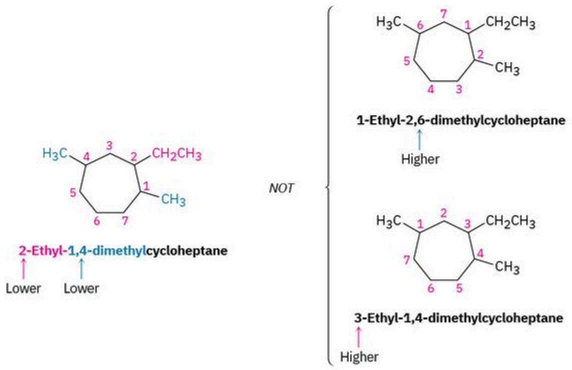


Figure 20.4g. Numbering the substituents on a cycloheptane by selecting the lower combination of numbers. (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0)

(a) When two or more different alkyl groups are present that could potentially take the same numbers, number them by alphabetical priority, ignoring numerical prefixes such as di- and tri-. An example is demonstrated in Figure 20.4h.

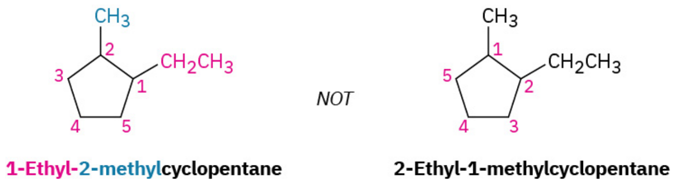


Figure 20.4h. Naming alkyl groups in alphabetical order within a cyclopentane (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0)

(b) If halogens are present, treat them just like alkyl groups as shown in Figure 20.4i.

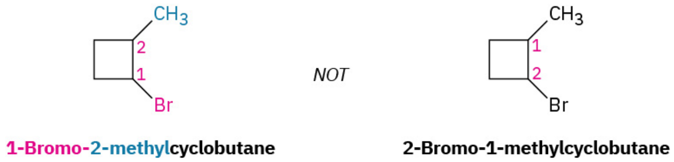


Figure 20.4i. Naming halogens like that of alkyl groups on a cyclobutane (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0)

Some additional examples that follow the IUPAC nomenclature system for cycloalkanes are demonstrated in Figure 20.4j.

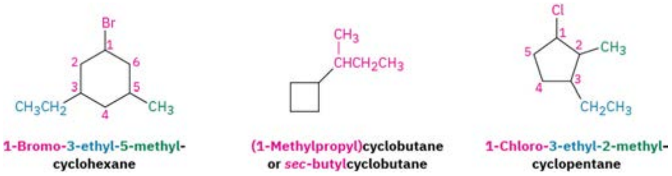
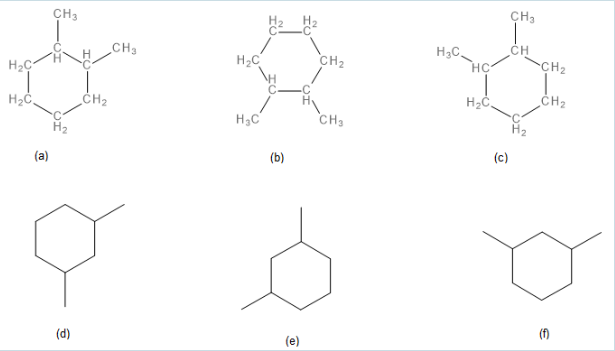


Figure 20.4j. Examples of additional substituted cycloalkanes (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0)

Exercise 20.4b

Name each structure.



Check Your Answers:[2]

Activity source: Exercise 20.4b is created by Samantha Sullivan Sauer, using images from Biovia Draw, licensed under CC BY-NC 4.0

Cis-Trans Isomerism of Cycloalkanes

In many respects, the chemistry of cycloalkanes is like that of open-chain alkanes: both are nonpolar and fairly inert. There are, however, some important differences. One difference is that cycloalkanes are less flexible than open-chain alkanes. In contrast with the relatively free rotation around single bonds in open-chain alkanes, there is much less freedom in cycloalkanes. Cyclopropane, for example, must be a rigid, planar molecule because three points (the carbon atoms) define a plane. No bond rotation can take place around a cyclopropane carbon–carbon bond without breaking open the ring as shown in Figure 20.4k.

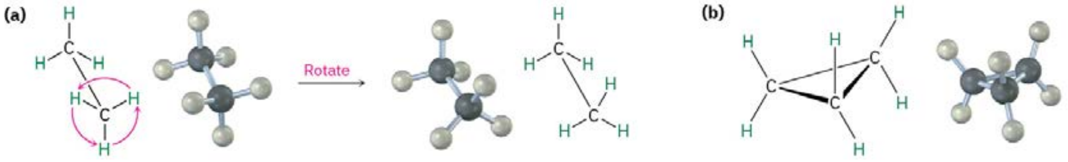
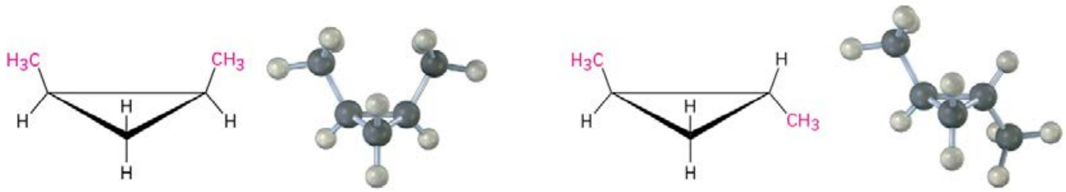


Figure 20.4k. Bond rotation in ethane and cyclopropane. **(a)** Rotation occurs around the carbon–carbon bond in ethane, but **(b)** no rotation is possible around the carbon–carbon bonds in cyclopropane without breaking open the ring.(credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0)

Larger cycloalkanes have increasing rotational freedom, and very large rings (C_{25} and up) are so floppy that they are nearly indistinguishable from open-chain alkanes. The common ring sizes (C_3–C_7), however, are severely restricted in their molecular motions.

Because of their cyclic structures, cycloalkanes have two faces when viewed edge-on, a “top” face and a “bottom” face. As a result, isomerism is possible in substituted cycloalkanes. For example, there are two different 1,2-dimethylcyclopropane isomers, one with the two methyl groups on the same face of the ring and one with the methyl groups on opposite faces as shown in Figure 20.4l. Both isomers are stable compounds, and neither can be converted into the other without breaking and reforming chemical bonds.



cis-1,2-Dimethylcyclopropane

trans-1,2-Dimethylcyclopropane

Figure 20.4l. There are two different 1,2-dimethylcyclopropane isomers, one with the methyl groups on the same face of the ring (cis) and the other with the methyl groups on opposite faces of the ring (trans). The two isomers do not interconvert (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0).

Unlike the constitutional isomers butane and isobutane, which have their atoms connected in a different order, the two 1,2-dimethylcyclopropanes have the same order of connections but differ in the spatial orientation of the atoms. Such compounds, with atoms connected in the same order but differing in three-dimensional orientation, are called stereochemical isomers, or stereoisomers. As we saw previously, the term stereochemistry is used generally to refer to the three-dimensional aspects of structure and reactivity. Figure 20.4m. demonstrates the difference between the types of isomers.

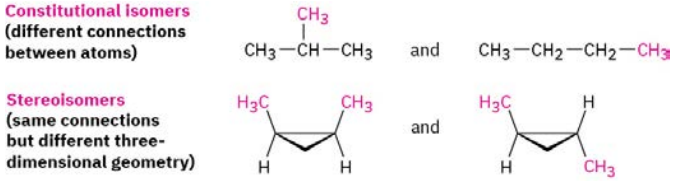


Figure 20.4m. The figure demonstrates the difference between constitutional isomers and stereoisomers (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0

The 1,2-dimethylcyclopropanes are members of a subclass of stereoisomers called cis–trans isomers as shown in Figure 20.4n. The prefixes *cis*– (Latin "on the same side") and *trans*– (Latin "across") are used to distinguish between them. Cis–trans isomerism is a common occurrence in substituted cycloalkanes and in many cyclic biological molecules.

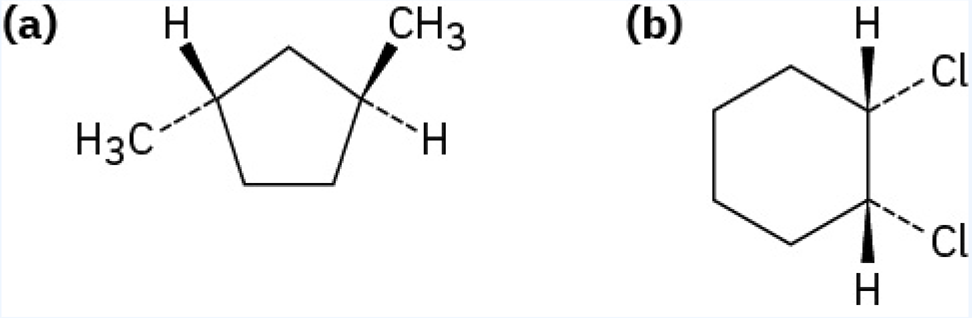
cis-**1,3-Dimethylcyclobutane** *trans*-**1-Bromo-3-ethylcyclopentane**

Figure 20.4n. The cis and trans isomers are shown through cis-1, 3-Dimethylcyclobutane and trans-1-Bromo-3-ethylcyclopentane (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0).

Example 20.4b

Naming Cycloalkanes

Name the following substances, including the *cis*– or *trans*– prefix:



(credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0)

Strategy

In these views, the ring is roughly in the plane of the page, a wedged bond protrudes out of the page, and a dashed bond recedes into the page. Two substituents are cis if they are both out of or both into the page, and they are trans if one is out of and one is into the page.

Solution

(a) *trans*-1,3-Dimethylcyclopentane

(b) *cis*-1,2-Dichlorocyclohexane

For a more in-depth look at cycloalkanes, watch the video Cyclohexanes as shown below.

Watch Cyclohexanes: Crash Course Organic Chemistry #7 – YouTube (14 min) (https://youtu.be/GRVxDqhgOYo?)

Spotlight on Everyday Chemistry: Carp and The Earthy Flavour Geosmin

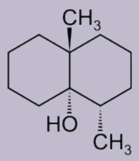


Figure 20.4o. The molecular structure of geosmin. (credit: Image by Xplus1, PDM).

Serving carp is common at Christmas in Europe. Thanks to the cycloalkane compound geosmin (Figure 20.4o), it gives the carp an earthly flavour. For more information see the infographic Compound Interest: The Chemistry Advent Calendar 2023 (compoundchem.com) (https://www.compoundchem.com/2023advent/#day3).

Attribution & References

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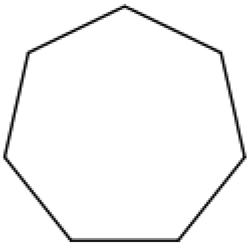
- "Ch. 4 Why This Chapter?", "4.1 Naming Cycloalkanes" and "4.2 Cis–Trans Isomerism in Cycloalkanes" In *Organic Chemistry (OpenStax)* licensed under CC BY-NC-SA 4.0. Access for free at *Organic Chemistry (OpenStax)* (https://openstax.org/books/organic-chemistry/)

Notes

1.  b. See the image: Ethylcyclohexane | C8H16 | CID 15504 - PubChem (nih.gov) (https://pubchem.ncbi.nlm.nih.gov/compound/ethylcyclohexane). **Image Source:** a. Image by Rhododendronbusch, PDM

2. Structures a, b, and c are the same. 1,2-dimethylcyclohexane. Structures d, e, and f are the same. 1,3-dimethylcyclohexane. Ring number start at the location that results in the lowest number for all substituents and can proceed in a clockwise or counterclockwise direction.

20.5 HALOGENATED ALKANES

Learning Objectives

By the end of this section, you will be able to:

- Name halogenated hydrocarbons given formulas and write formulas for these compounds given names.

Halogenated Alkanes

Many organic compounds are closely related to the alkanes. As we noted previously, alkanes react with halogens to produce halogenated hydrocarbons, the simplest of which have a single halogen atom substituted for a hydrogen atom of the alkane. Even more closely related are the cycloalkanes, compounds in which the carbon atoms are joined in a ring, or cyclic fashion.

Halogens are found in column 7A of the periodic table and include Fluorine, Chlorine, Bromine and Iodine. Refer to Appendix A: Key Element Information for more details about halogens.

Figure 20.5a. The gases released during volcanic eruptions contain large amounts of organohalides, including chloromethane, chloroform, dichlorodifluoromethane, and many others. (credit: modification of "Tavurvur volcano" by Taro Taylor (https://www.flickr.com/photos/30674396@N00) edit by Richard Bartz, CC BY 2.0).

Alkyl halides are encountered less frequently than their oxygen-containing relatives and are not often involved in the biochemical pathways of terrestrial organisms, but some of the kinds of reactions they undergo—nucleophilic substitutions and eliminations—are encountered frequently. Thus, alkyl halide chemistry is a relatively simple model for many mechanistically similar but structurally more complex reactions found in biomolecules.

Now that we've covered the chemistry of hydrocarbons, it's time to start looking at more complex substances that contain elements in addition to C and H. We'll begin by discussing the chemistry of organohalides, compounds that contain one or more halogen atoms.

Halogen-substituted organic compounds are widespread in nature, and more than 5000 organohalides have been found in algae and various other marine organisms. Chloromethane, for instance, is released in large amounts by ocean kelp, as well as by forest fires and volcanoes. Halogen-containing compounds also have an array of industrial applications, including their use as solvents, inhaled anesthetics in medicine, refrigerants, and pesticides as shown in Figure 20.5b.

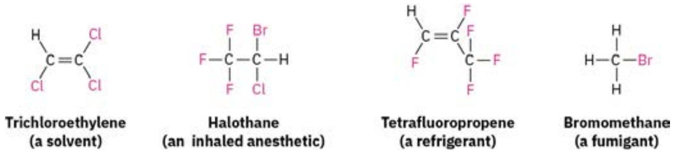
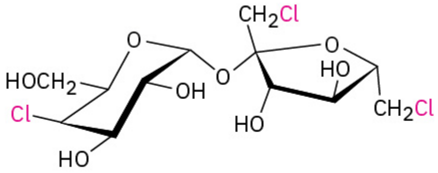


Figure 20.5b. Examples of halogen containing compounds trichloroethylene (a solvent), halothane (an inhaled anesthetic), tetrafluoropropene (a refrigerant), and bromomethane (a fumigant) (credit: *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/10-why-this-chapter)*, CC BY-NC-SA 4.0).

Still other halo-substituted compounds are used as medicines and food additives. The nonnutritive sweetener sucralose, marketed as Splenda, contains three chlorine atoms, for instance. Sucralose is about 600 times as sweet as sucrose, so only 1 mg is equivalent to an entire teaspoon of table sugar. Refer to Figure 20.5c. for the structural formula of sucralose.



Sucralose

Figure 20.5c. Structural formula of sucralose (credit: *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/10-why-this-chapter)*, CC BY-NC-SA 4.0).

A large variety of organohalides are known. The halogen might be bonded to an alkynyl group (C≡C−X), a vinylic group (C═C–XC═C–X">C═C–X), an aromatic ring (Ar–X), or an alkyl group.

The reactions of alkanes with halogens produce halogenated hydrocarbons, compounds in which one or more hydrogen atoms of a hydrocarbon have been replaced by halogen atoms (F, Cl, Br and I):

CH_3CH_2Cl $CH_3CHBrCH_2Br$ CH_3CHICH_2Cl

Figure 20.5d. Condensed formulas of halogenated compounds involving chlorine and bromine atoms. (Credit: *Introduction to Chemistry: GOB (V. 1.0)*. ,CC BY-NC-SA 3.0.)

The replacement of only one hydrogen atom gives an alkyl halide (or haloalkane) as shown in Figure 20.5d. above.

Indigenous Perspectives: The Impact of Fluorocarbons on Inuit People of Canada

The long-chained fluorocarbon ending with a -SO_3H group is known as perfluorooctanesulfonic acid also known as PFOS (Figure 20.5e.). PFOS and their relatives contain a long fluorocarbon backbone that is extremely resistant to decomposition. In addition, the PFOS family of compounds are volatile and can spread throughout the Earth's surface. Research has shown that through global distillation, these PFOS have accumulated in the Arctic. This is a problematic health concern for the Inuit in the north. Several food sources that are part of the Inuit diet have been tested and contain PFOS. Exposure to PFOS have numerous health implications such as cancer, endocrine delays and others as described in the article below. There is no end in sight from exposure to these harmful fluorocarbons as they are expected to remain in the arctic for hundreds and possibly thousands of years (Anderson & Rayner-Canham, 2022).

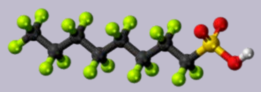


Figure 20.5e. The ball-and-stick model of perfluorooctanesulfonic acid. (credit: Image by Jynto, CC0)

For more detailed information regarding the fluorocarbons and their impact on the Inuit see the following link: PFOS | Chem 13 News Magazine | University of Waterloo (uwaterloo.ca) (https://uwaterloo.ca/chem13-news-magazine/fall-2022-special-edition/feature/pfos).

Naming Haloalkanes

Although commonly called *alkyl halides*, halogen-substituted alkanes are named systematically as *haloalkanes*, treating the halogen as a substituent on a parent alkane chain. There are three steps:

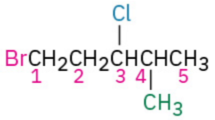
1. Find the longest chain, and name it as the parent. If a double or triple bond is present, the parent chain must contain it.
2. Number the carbons of the parent chain beginning at the end nearer the first substituent, whether alkyl or halo. Assign each substituent a number according to its position on the chain. Figure 20.5f. provides two examples on how to number the carbon chain with either an alkyl or halo first appearing in the chain.

$CH_3CHCH_2CHCHCH_2CH_3$ $CH_3CHCH_2CHCHCH_2CH_3$

5-Bromo-2,4-dimethylheptane **2-Bromo-4,5-dimethylheptane**

Figure 20.5f. Numbering the carbon chain using 5-Bromo-2,4-dimethylheptane and 2-Bromo-4,5-deimethylheptane as examples (credit: *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/10-1-names-and-structures-of-alkyl-halides)*, CC BY-NC-SA 4.0).

3. If different halogens are present, number each one and list them in alphabetical order when writing the name as shown in Figure 20.5g.

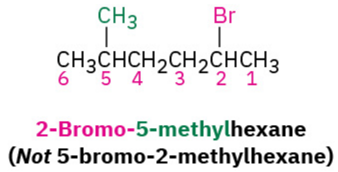


$BrCH_2CH_2CHCHCH_3$

1-Bromo-3-chloro-4-methylpentane

Figure 20.5g. Numbering the carbon chain 1-Bromo-3-chloro-4-methylpentane (credit: *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/10-1-names-and-structures-of-alkyl-halides)*, CC BY-NC-SA 4.0).

4. If the parent chain can be properly numbered from either end by step 2, begin at the end nearer the substituent that has alphabetical precedence. Figure 20.5h. shows an example of alphabetical precedence.



$$\overset{CH_3}{|}\qquad\overset{Br}{|}$$
$$CH_3CHCH_2CH_2CHCH_3$$

Figure 20.5h. An example of alphabetical precedence of 2-Bromo-5-methylhexane (credit: *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/10-1-names-and-structures-of-alkyl-halides),* CC BY-NC-SA 4.0).

5. In addition to their systematic names, many simple alkyl halides are also named by identifying first the alkyl group and then the halogen. For example in Figure 20.5i., CH3I can be called either iodomethane or methyl iodide. Such names are well entrenched in the chemical literature and in daily usage, but they won't be used in this book.

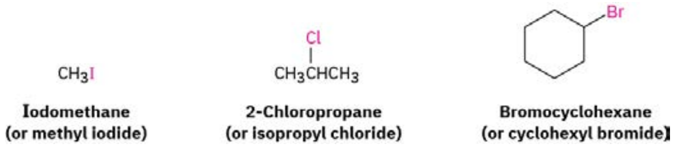
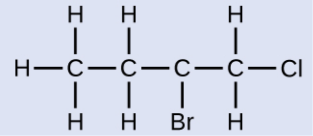


Figure 20.5i. Naming alkyl halides iodomethane, 2-chloropropane and bromocyclohexane (credit: *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/10-1-names-and-structures-of-alkyl-halides)*, CC BY-NC-SA 4.0).

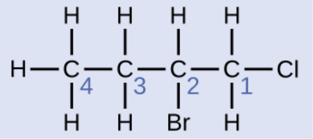
In summary, the *common names* of alkyl halides consist of two parts: the name of the alkyl group plus the stem of the name of the halogen, with the ending *-ide*. The IUPAC system uses the name of the parent alkane with a prefix indicating the halogen substituents, preceded by number indicating the substituent's location. The prefixes are *fluoro-*, *chloro-*, *bromo-*, and *iodo-*. Thus CH_3CH_2Cl has the common name ethyl chloride and the IUPAC name chloroethane. Alkyl halides with simple alkyl groups (one to four carbon atoms) are often called by common names. Those with a larger number of carbon atoms are usually given IUPAC names.

Example 20.5a

Name the molecule whose structure is shown here:



Solution

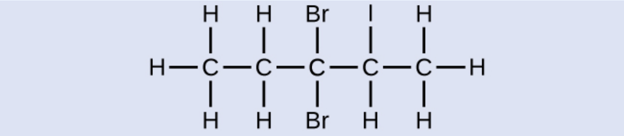


The four-carbon chain is numbered from the end with the chlorine atom. This puts the substituents on positions 1 and 2 (numbering from the other end would put the substituents on positions 3 and 4). Four carbon atoms means that the base name of this compound will be butane. The bromine at position 2 will be described by adding 2-bromo-; this will come at the beginning of the name, since bromo- comes before chloro- alphabetically. The chlorine at position 1 will be described by adding 1-chloro-, resulting in the name of the molecule being 2-bromo-1-chlorobutane.

Example & image source: *General Chemistry 1 & 2* , CC BY 4.0.

Example 20.5b

Name the following molecule:



Solution

3,3-dibromo-2-iodopentane

Example & image source: *General Chemistry 1 & 2* , CC BY 4.0.

Example 20.5c

Give the common and IUPAC names for each compound.

a. $CH_3CH_2CH_2Br$
b. $(CH_3)_2CHCl$

Solution

a. The alkyl group ($CH_3CH_2CH_2$–) is a propyl group, and the halogen is bromine (Br). The common name is therefore propyl bromide. For the IUPAC name, the prefix for bromine (bromo) is combined with the name for a three-carbon chain (propane), preceded by a number identifying the carbon atom to which the Br atom is attached, so the IUPAC name is 1-bromopropane.
b. The alkyl group [$(CH_3)_2CH$–] has three carbon atoms, with a chlorine (Cl) atom attached to the middle carbon atom. The alkyl group is therefore isopropyl, and the common name of the compound is isopropyl chloride. For the IUPAC name, the Cl atom (prefix *chloro*-) attached to the middle (second) carbon atom of a propane chain results in 2-chloropropane.

Exercise 20.5a

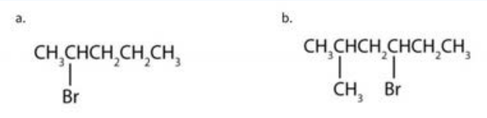
Give common and IUPAC names for each compound.

a. CH_3CH_2I
b. $CH_3CH_2CH_2CH_2F$

Check Your Answer [1]

Example 20.5d

Give the IUPAC name for each compound.



a. $CH_3\underset{\underset{Br}{|}}{C}HCH_2CH_2CH_3$

b. $CH_3\underset{\underset{CH_3}{|}}{C}HCH_2\underset{\underset{Br}{|}}{C}HCH_2CH_3$

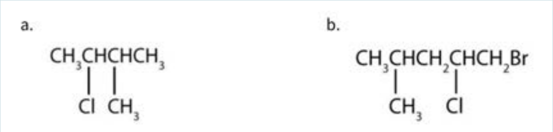
(credit: *Intro Chem: GOB(V. 1.0).* ,CC BY-NC-SA 3.0.)

Solution

1. The parent alkane has five carbon atoms in the longest continuous chain; it is pentane. A bromo (Br) group is attached to the second carbon atom of the chain. The IUPAC name is 2-bromopentane.
2. The parent alkane is hexane. Methyl (CH_3) and bromo (Br) groups are attached to the second and fourth carbon atoms, respectively. Listing the substituents in alphabetical order gives the name 4-bromo-2-methylhexane.

Exercise 20.5b

Give the IUPAC name for each compound.



(Credit: *Intro Chem: GOB (V. 1.0).* ,CC BY-NC-SA 3.0.)

Check Your Answer[2]

For an overview on how to name alkyl halides, watch the video Naming Alkyl Halides – IUPAC Nomenclature below.

Watch Naming Alkyl Halides – IUPAC Nomenclature – YouTube (12 min) (https://youtu.be/595ENX3iqEE?)

A wide variety of interesting and often useful compounds have one or more halogen atoms per molecule. For example, methane (CH_4) can react with chlorine (Cl_2), replacing one, two, three, or all four hydrogen atoms with Cl atoms. Several halogenated products derived from methane and ethane (CH_3CH_3) are listed in Table 20.5a., along with some of their uses.

Table 20.5a. Some Halogenated Hydrocarbons

Formula	Derived from	Common Name	IUPAC Name	Some Important Use
CH_3Cl	CH_4	methyl chloride	chloromethane	refrigerant; the manufactu silicones, methyl cellulose, synthetic rubber
CH_2Cl_2	CH_4	methylene chloride	dichloromethane	laboratory and industrial sc
$CHCl_3$	CH_4	chloroform	trichloromethane	industrial solvent
CCl_4	CH_4	carbon tetrachloride	tetrachloromethane	dry-cleaning solvent and extinguishers (but no lon recommended for use)
$CBrF_3$	CH_4	halon-1301	bromotrifluoromethane	fire extinguisher system
CCl_3F	CH_4	chlorofluorocarbon-11 (CFC-11)	trichlorofluoromethane	foaming plastics
CCl_2F_2	CH_4	chlorofluorocarbon-12 (CFC-12)	dichlorodifluoromethane	refrigerant
CH_3CH_2Cl	CH_3CH_3	ethyl chloride	chloroethane	local anesthetic
$ClCH_2CH_2Cl$	CH_3CH_3	ethylene dichloride	1,2-dichloroethane	solvent for rubber
CCl_3CH_3	CH_3CH_3	methylchloroform	1,1,1-trichloroethane	solvent for cleaning compute and molds for shaping pla

Table source: "12.8: Halogenated Hydrocarbons" In *Basics of GOB Chemistry (Ball et al.)*, CC BY-NC-SA 4.0.

Alkyl halides can be both harmful and beneficial to your health. In the next examples, To Your Health and Spotlight in Chemistry you can learn more about these interesting compounds.

Spotlight on Everyday Chemistry: Halogenated Hydrocarbons Risks and Benefits

Once widely used in consumer products, many chlorinated hydrocarbons are suspected carcinogens (cancer-causing substances) and also are known to cause severe liver damage. An example is carbon tetrachloride (CCl_4), once used as a dry-cleaning solvent and in fire extinguishers but no longer recommended for either use. Even in small amounts, its vapor can cause serious illness if exposure is prolonged. Moreover, it reacts with water at high temperatures to form deadly phosgene ($COCl_2$) gas, which makes the use of CCl_4 in fire extinguishers particularly dangerous.

Ethyl chloride, in contrast, is used as an external local anesthetic. When sprayed on the skin, it evaporates quickly, cooling the area enough to make it insensitive to pain. It can also be used as an emergency general anesthetic.

Bromine-containing compounds are widely used in fire extinguishers and as fire retardants on clothing and other materials. Because they too are toxic and have adverse effects on the environment, scientists are engaged in designing safer substitutes for them, as for many other halogenated compounds.

Halomon (IUPAC name (3*S*,6*R*)-6-Bromo-3-(bromomethyl)-2,3,7-trichloro-7-methyloct-1-ene) is a pentahalogenated alkene. Halomon as shown in Figure 20.5j., has been isolated from the red alga *Portieria hornemannii* and found to have anticancer activity against several human tumor cell lines.

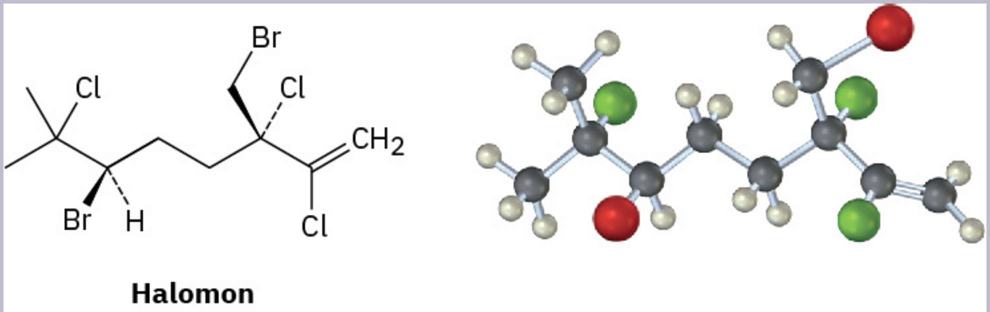


Figure 20.5j. Chemical structure of halomon (credit: *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/10-chemistry-matters-naturally-occurring-organohalides)*, CC BY-NC-SA 4.0).

Links to Enhanced Learning

For more examples, visit Haloalkanes (https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Organic_Chemistry_I_(Cortes)/07%3A_Introduction_to_Organic_Chemistry/7.04%3A_Haloalkanes_or_Alkyl_Halides) and Names and Properties of Alkyl Halides (https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Organic_Chemistry_(Morsch_et_al.)/10%3A_Organohalides/10.01%3A_Names_and_Properties_of_Alkyl_Halides) by LibreTextsChemistry.

Attribution & References

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- "18.1 Hydrocarbons (https://boisestate.pressbooks.pub/chemistry/chapter/21-1-hydrocarbons/)" In *General Chemistry 1 & 2* by Rice University, a derivative of *Chemistry (Open Stax)* by Paul Flowers, Klaus Theopold, Richard Langley & William R. Robinson and is licensed under CC BY 4.0. Access for free at *Chemistry (OpenStax) (https://openstax.org/books/chemistry/pages/1-introduction)*
- "12.8: Halogenated Hydrocarbons" In *Basics of General, Organic, and Biological Chemistry (Ball et al.)* by David W. Ball, John W. Hill, and Rhonda J. Scott via LibreTexts, licensed under CC BY-NC-SA 4.0. / A derivative of *Introduction to Chemistry: GOB (v. 1.0),* CC BY-NC 3.0.
- "10.1 Names and Structures of Alkyl Halides" and "Chemistry Matters—Naturally Occurring Organohalides" In *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/1-why-this-chapter)* by John McMurray, CC BY-NC-SA 4.0. Access for free at *Organic Chemistry (OpenStax) (https://openstax.org/books/organic-chemistry/pages/1-why-this-chapter)*

References cited in-text

Anderson, C. C., & Rayner-Canham, G. (2022, Fall). PFOS: The newest Arctic pollutant (https://uwaterloo.ca/chem13-news-magazine/fall-2022-special-edition/feature/pfos). *Chem 13 News Magazine.*

Notes

1.
    a. 1-Iodoethane
    b. 1-Fluorobutane
2.
    a. 2-chloro, 3-methylbutane
    b. 1-bromo, 2-chloro, 4-methylpentane

20.6 REACTIONS OF ALKANES

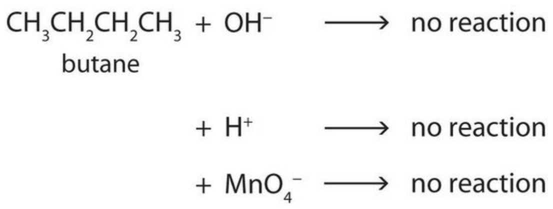
Learning Objectives

By the end of this section, you will be able to:

- Understand the reactions of alkanes: combustion and substitution.

Reactions of Alkanes

Alkane molecules are nonpolar and therefore generally do not react with ionic compounds such as most laboratory acids, bases, oxidizing agents, or reducing agents. Consider butane as an example in Figure 20.6a.



$$\underset{\text{butane}}{CH_3CH_2CH_2CH_3} + OH^- \longrightarrow \text{no reaction}$$

$$+ H^+ \longrightarrow \text{no reaction}$$

$$+ MnO_4^- \longrightarrow \text{no reaction}$$

Figure 20.6a. Butane plus O H superscript negative sign yields no reaction. There is also no reaction of butane with H superscript positive sign and Mn O subscript 4 superscript negative sign. (Credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 4.0.)

Neither positive ions nor negative ions are attracted to a nonpolar molecule. In fact, the alkanes undergo so few reactions that they are sometimes called *paraffins*, from the Latin *parum affinis*, meaning “little affinity.”

However, heat or light can initiate the breaking of C–H or C–C single bonds in reactions called **combustion** and **substitution**.

Watch Alkanes: Crash Course Organic Chemistry #6 – YouTube (12 min) (https://youtu.be/ryHnC0wqTTo?)

Recall that organic functional groups can be converted into other functional groups through reactions. A map of some of the more common reactions to convert functional groups can be found in Section 19.6 – General Reactions of Carbon in Infographic 19.6a.

Combustion

Alkanes are relatively stable molecules, but heat or light will activate reactions that involve the breaking of C–H or C–C single bonds. Combustion is one such reaction:

$$\mathrm{CH_4}(g) \; + \; 2\mathrm{O_2}(g) \longrightarrow \mathrm{CO_2}(g) \; + \; 2\mathrm{H_2O}(g)$$

Alkanes burn in the presence of oxygen, a highly exothermic oxidation-reduction reaction that produces carbon dioxide and water. As a consequence, alkanes are excellent fuels. For example, methane, CH_4, is the principal component of natural gas. Butane, C_4H_{10}, used in camping stoves and lighters is an alkane. Gasoline is a liquid mixture of continuous- and branched-chain alkanes, each containing from five to nine carbon atoms, plus various additives to improve its performance as a fuel. Kerosene, diesel oil, and fuel oil are primarily mixtures of alkanes with higher molecular masses. The main source of these liquid alkane fuels is crude oil, a complex mixture that is separated by fractional distillation. Fractional distillation takes advantage of differences in the boiling points of the components of the mixture (see Figure 20.6b.). You may recall that boiling point is a function of intermolecular interactions.

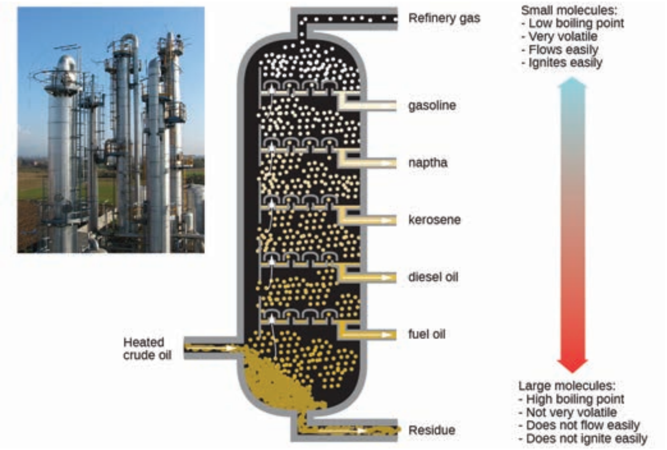


Figure 20.6b. In a column for the fractional distillation of crude oil, oil heated to about 425 °C in the furnace vaporizes when it enters the base of the tower. The vapors rise through bubble caps in a series of trays in the tower. As the vapors gradually cool, fractions of higher, then of lower, boiling points condense to liquids and are drawn off. (credit left: modification of work by Luigi Chiesa, CC BY 3.0, right: *General Chemistry 1 & 2*, CC BY 4.0)

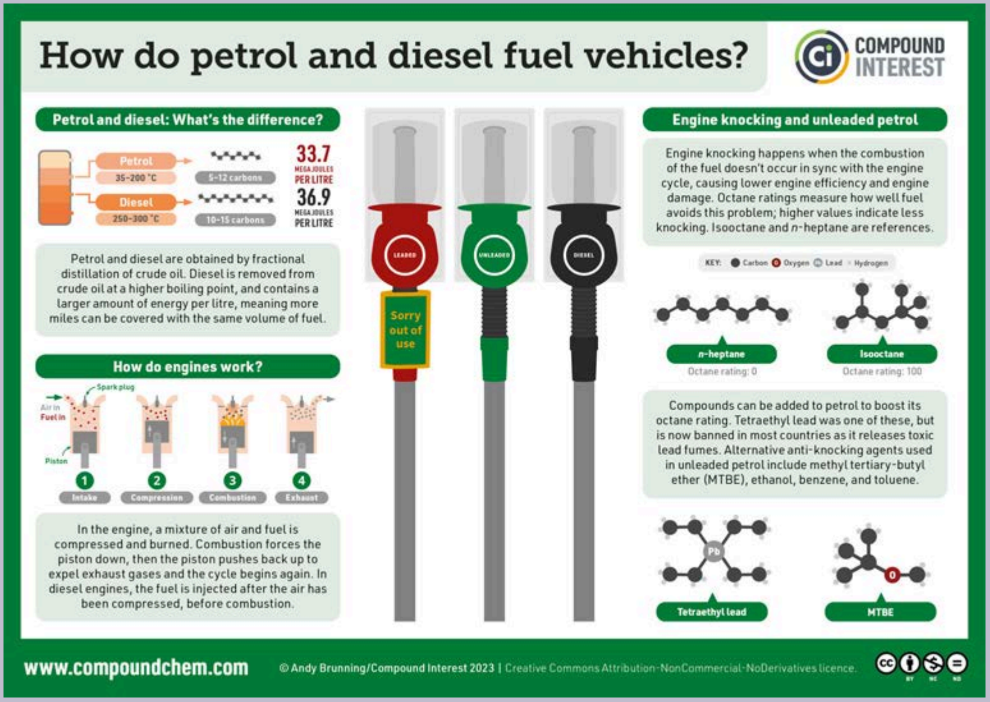
If the reactants of combustion reactions are adequately mixed, and there is sufficient oxygen, the only products are carbon dioxide (CO_2), water (H_2O), and energy—heat for cooking foods, heating homes, and drying clothes. Because conditions are rarely ideal, other unwanted by-products are frequently formed. When the oxygen supply is limited, carbon monoxide (CO) is a by-product:

$$2CH_4 + 3O_2 \rightarrow 2CO + 4H_2O\label{2}$$

This reaction is responsible for dozens of deaths each year from unventilated or improperly adjusted gas heaters. (Similar reactions with similar results occur with kerosene heaters.)

Spotlight on Everyday Chemistry: Fuel

We use fuel (or petrol in the UK) in our vehicles everyday. Fuel comes from fossil fuels. Read more about how fuel works in Infographic 20.6a.



Petrol and diesel are obtained by fractional distillation of crude oil. Diesel is removed from crude oil at a higher boiling point, and contains a larger amount of energy per litre, meaning more miles can be covered with the same volume of fuel.

In the engine, a mixture of air and fuel is compressed and burned. Combustion forces the piston down, then the piston pushes back up to expel exhaust gases and the cycle begins again. In diesel engines, the fuel is injected after the air has been compressed, before combustion.

Engine knocking happens when the combustion of the fuel doesn't occur in sync with the engine cycle, causing lower engine efficiency and engine damage. Octane ratings measure how well fuel avoids this problem; higher values indicate less knocking. Isooctane and *n*-heptane are references.

Compounds can be added to petrol to boost its octane rating. Tetraethyl lead was one of these, but is now banned in most countries as it releases toxic lead fumes. Alternative anti-knocking agents used in unleaded petrol include methyl tertiary-butyl ether (MTBE), ethanol, benzene, and toluene.

Infographic 20.6a. Read more about "The Chemistry of Petrol & The Tetraethyl Lead Story (https://www.compoundchem.com/2016/05/17/petrol/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary of infographic 20.6a [New tab].

Substitution

In a substitution reaction (ex. halogenation), another typical reaction of alkanes, one or more of the alkane's hydrogen atoms is replaced with a different atom or group of atoms. No carbon-carbon bonds are broken in these reactions, and the hybridization of the carbon atoms does not change. For example in Figure 20.6c., the reaction between ethane and molecular chlorine demonstrates a substitution reaction.

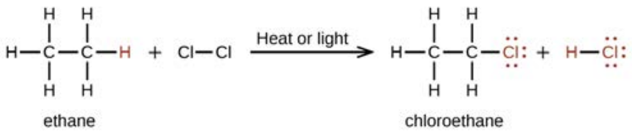


Figure 20.6c. Substitution reaction between ethane and chlorine to produce chloroethane and HCl. (credit: *General Chemistry 1 & 2*, CC BY 4.0)

The C–Cl portion of the chloroethane molecule is an example of a **functional group**, the part or moiety of a molecule that imparts a specific chemical reactivity. The types of functional groups present in an organic molecule are major determinants of its chemical properties and are used as a means of classifying organic compounds as detailed in the remaining sections of this chapter.

A wide variety of interesting and often useful compounds have one or more halogen atoms per molecule. For example, methane (CH_4) can react with chlorine (Cl_2), replacing one, two, three, or all four hydrogen atoms with Cl atoms. With more chlorine, a mixture of products is obtained: CH_3Cl, CH_2Cl_2, $CHCl_3$, and CCl_4. Fluorine (F), the lightest halogen, combines explosively with most hydrocarbons. Iodine (I) is relatively unreactive. Fluorinated and iodinated alkanes are produced by indirect methods.

Several halogenated products derived from methane and ethane (CH_3CH_3) are listed in Table 20.6a., along with some of their uses.

Table 20.6a. Some Halogenated Hydrocarbons

Formula	Common Name	IUPAC Name	Some Important Uses
		Derived from CH_4	
CH_3Cl	methyl chloride	chloromethane	refrigerant; the manufacture of silicones, methyl cellulose, and synthetic rubber
CH_2Cl_2	methylene chloride	dichloromethane	laboratory and industrial solvent
$CHCl_3$	chloroform	trichloromethane	industrial solvent
CCl_4	carbon tetrachloride	tetrachloromethane	dry-cleaning solvent and fire extinguishers (but no longer recommended for use)
$CBrF_3$	halon-1301	bromotrifluoromethane	fire extinguisher systems
CCl_3F	chlorofluorocarbon-11 (CFC-11)	trichlorofluoromethane	foaming plastics
CCl_2F_2	chlorofluorocarbon-12 (CFC-12)	dichlorodifluoromethane	refrigerant
		Derived from CH_3CH_3	
CH_3CH_2Cl	ethyl chloride	chloroethane	local anesthetic
$ClCH_2CH_2Cl$	ethylene dichloride	1,2-dichloroethane	solvent for rubber
CCl_3CH_3	methylchloroform	1,1,1-trichloroethane	solvent for cleaning computer chips and molds for shaping plastics

Table source: *Map: Fundamentals of GOB Chemistry (McMurry et al.),* CC BY-NC-SA 3.0.

Spotlight on Everyday Chemistry: Chlorofluorocarbons (CFC's), The Ozone Layer and Susan Solomon

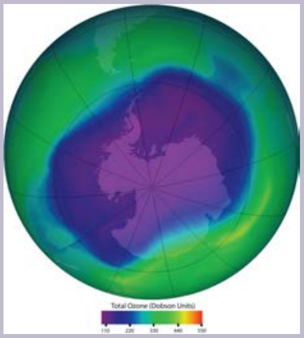


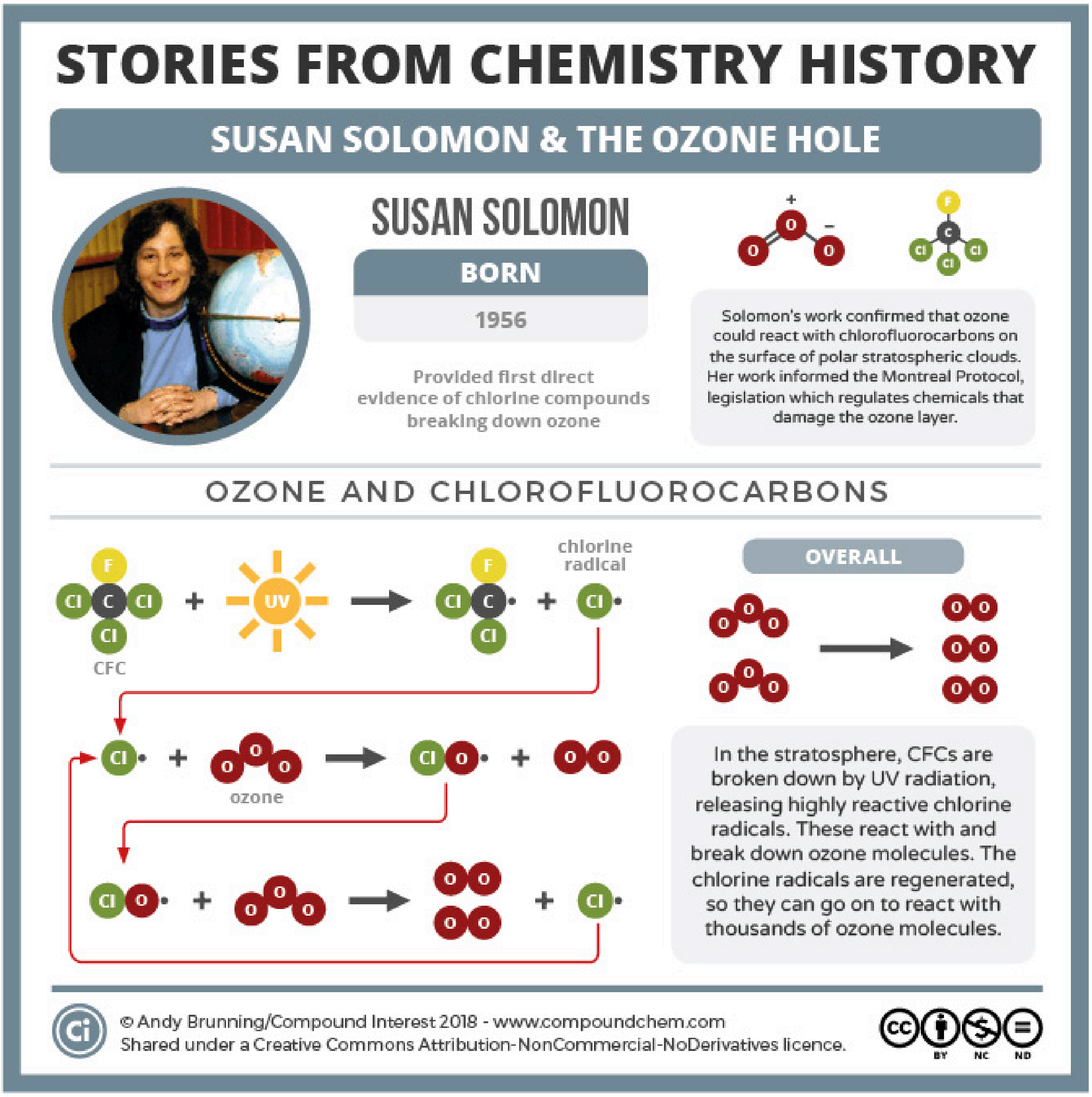
Figure 20.6d. Ozone in the upper atmosphere shields Earth's surface from UV radiation from the sun, which can cause skin cancer in humans and is also harmful to other animals and to some plants. Ozone "holes" in the upper atmosphere (the gray, pink, and purple areas at the center) are large areas of substantial ozone depletion. They occur mainly over Antarctica from late August through early October and fill in about mid-November. Ozone depletion has also been noted over the Arctic regions. The largest ozone hole ever observed occurred on 24 September 2006. (credit: NASA Ozone Watch, PDM, edited by Anonymous)

Chlorofluorocarbons and the Ozone Layer

Alkanes substituted with both fluorine (F) and chlorine (Cl) atoms have been used as the dispersing gases in aerosol cans, as foaming agents for plastics, and as refrigerants. Two of the best known of these chlorofluorocarbons (CFCs) are listed in Table 20.6a.

Chlorofluorocarbons contribute to the greenhouse effect in the lower atmosphere. They also diffuse into the stratosphere, where they are broken down by ultraviolet (UV) radiation to release Cl atoms. These in turn break down the ozone (O_3) molecules that protect Earth from harmful UV radiation as shown in Figure 20.6d. Worldwide action has reduced the use of CFCs and related compounds. The CFCs and other Cl- or bromine (Br)-containing ozone-destroying compounds are being replaced with more benign substances. Hydrofluorocarbons (HFCs), such as CH_2FCF_3, which have no Cl or Br to form radicals, are one alternative. Another is hydrochlorofluorocarbons (HCFCs), such as $CHCl_2CF_3$. HCFC molecules break down more readily in the troposphere, and fewer ozone-destroying molecules reach the stratosphere.

Thanks to Susan Solomon as described in infographic 20.6b, she confirmed that ozone could react with CFC's in the stratosphere breaking it down..



Provided first direct evidence of chlorine compounds breaking down ozone

Solomon's work confirmed that ozone could react with chlorofluorocarbons on the surface of polar stratospheric clouds. Her work informed the Montreal Protocol, legislation which regulates chemicals that damage the ozone layer.

In the stratosphere, CFCs are broken down by UV radiation, releasing highly reactive chlorine radicals. These react with and break down ozone molecules. The chlorine radicals are regenerated, so they can go on to react with thousands of ozone molecules.

Infographic 20.6b. Read more about "Today in Chemistry History: Susan Solomon, ozone depletion, and CFCs (https://www.compoundchem.com/2018/01/19/solomon-cfcs/)" by Andy Brunning / Compound Interest, CC BY-NC-ND, or access a text-based summary of infographic 20.6b [New tab]

For more information on reactions of alkanes, watch Radical Reactions & Hammond's Postulate below.

Watch Radical Reactions & Hammond's Postulate: Crash Course Organic Chemistry #19 – YouTube (12 min) (https://youtu.be/WsKWFoIMCQ0?)

Cracking (Elimination) – Making Alkenes

Ethylene and propylene, the simplest alkenes, are the two most important organic chemicals produced industrially. Approximately 220 million tons of ethylene and 138 million tons of propylene are produced worldwide each year for use in the synthesis of polyethylene, polypropylene, ethylene glycol, acetic acid, acetaldehyde, and a host of other substances (Figure 20.6e.).

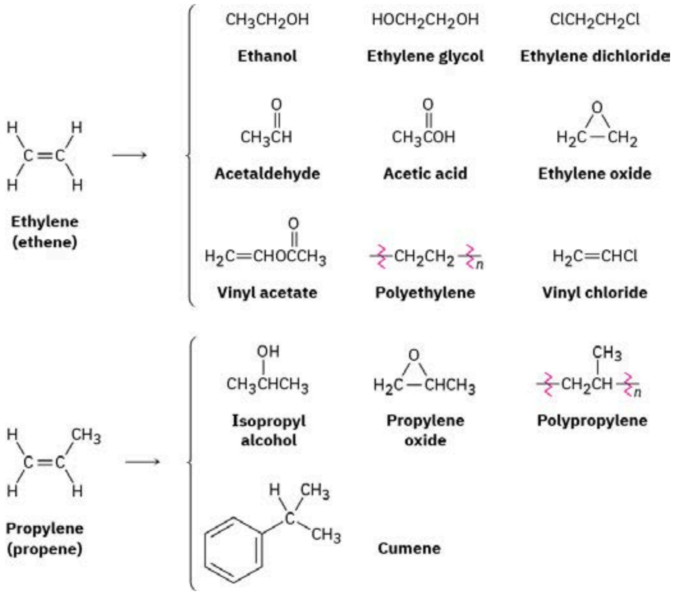


Figure 20.6e. Compounds derived industrially from ethylene and propylene. (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0).

Ethylene, propylene, and butene are synthesized from (C_2–C_8) alkanes by a process called *steam cracking* at temperatures up to 900 °C. This process is shown in Figure 20.6f. below.

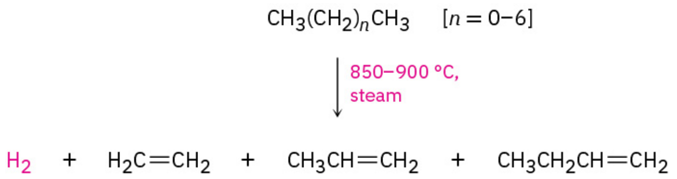


Figure 20.6f. Steam cracking of Ethylene, propylene, and butene at high temperatures of 900^{o}C. (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0).

The cracking process is complex, although it undoubtedly involves radical reactions. The high-temperature reaction conditions cause spontaneous breaking of C–C and C–H bonds, with the resultant formation of smaller fragments. We might imagine, for instance, that a molecule of butane splits into two ethyl radicals, each of which then loses a hydrogen atom to generate two molecules of ethylene as demonstrated in Figure 20.6g.

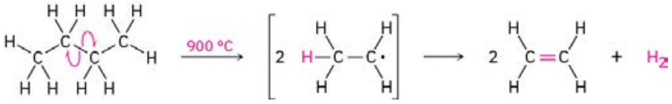


Figure 20.6g. Butane undergoes cracking and creates two molecules of ethylene. (credit: *Organic Chemistry (OpenStax)*, CC BY-NC-SA 4.0).

Other Alkane Reactions

Two additional alkane reactions include dehydrogenation and isomerization. **Dehydrogenation** is an elimination reaction where a hydrogen is lost from an alkane to create an alkene under high temperatures. The results are a by-product of hydrogen gas and an alkene. This reaction is unpredictable as the location of the carbon-carbon double bond is random. The dehydrogenation process is used in the production of motor fuels and petrochemicals (Hein et al., 2013, p. 464). The dehydrogenation reaction of butane is shown in Figure 20.6h.

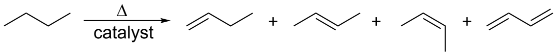


Figure 20.6h. Dehydrogenation of butane resulting in a mixture of butene compounds (credit: Image by Hbf878, CC0).

Isomerization occurs when there is a rearrangement of the molecular structure under heat, pressure and exposure to a catalyst. Again, this process is used in the production of motor fuels and petrochemicals (Hein et al., 2013, p. 464). For example, in Figure 20.6i., the isomerization of butane is demonstrated.

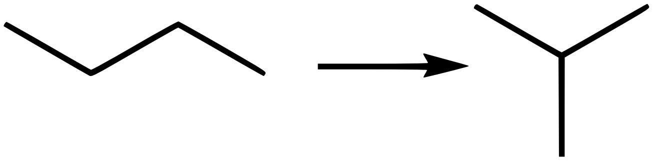


Figure 20.6i. The isomerization reaction of butane to produce 2-methylpropane using heat and a catalyst (credit: Image by Smokefoot, CC0).

For more details on reactions involving alkanes refer to the map of some of the more common reactions to convert functional groups in Section 19.6 – General Reactions of Carbon in Infographic 19.6a.

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References cited in-text

Hein, M., Pattison, S., Arena, S., & Best, L. (2013). *Introduction to general, organic, and biochemistry* (11th ed.). John Wiley & Sons, Inc.

CHAPTER 20 - SUMMARY

20.1 Characteristics of Alkanes

Organic chemistry is the chemistry of carbon compounds, and inorganic chemistry is the chemistry of all the other elements. Carbon atoms can form stable covalent bonds with other carbon atoms and with atoms of other elements, and this property allows the formation the tens of millions of organic compounds. Hydrocarbons contain only hydrogen and carbon atoms.

Hydrocarbons in which each carbon atom is bonded to four other atoms are called alkanes or saturated hydrocarbons. They have the general formula C_nH_{2n+2}. Any given alkane differs from the next one in a series by a CH_2 unit. Any family of compounds in which adjacent members differ from each other by a definite factor is called a homologous series.

20.2 Isomers and Nomenclature of Alkanes

Carbon atoms in alkanes can form straight chains or branched chains. Two or more compounds having the same molecular formula but different structural formulas are isomers of each other. There are no isomeric forms for the three smallest alkanes; beginning with C_4H_{10}, all other alkanes have isomeric forms.

A structural formula shows all the carbon and hydrogen atoms and how they are attached to one another. A condensed structural formula shows the hydrogen atoms right next to the carbon atoms to which they are attached. A line formula is a formula in which carbon atoms are implied at the corners and ends of lines. Each carbon atom is understood to be attached to enough hydrogen atoms to give each carbon atom four bonds.

The IUPAC System of Nomenclature provides rules for naming organic compounds. An alkyl group is a unit formed by removing one hydrogen atom from an alkane.

The physical properties of alkanes reflect the fact that alkane molecules are nonpolar. Alkanes are insoluble in water and less dense than water.

20.3 Cycloalkanes

Cycloalkanes are hydrocarbons whose molecules are closed rings rather than straight or branched chains. A cyclic hydrocarbon is a hydrocarbon with a ring of carbon atoms.

20.4 Halogenated Alkanes

Alkanes react with halogens by substituting one or more halogen atoms for hydrogen atoms to form halogenated hydrocarbons. An alkyl halide (haloalkane) is a compound resulting from the replacement of a hydrogen atom of an alkane with a halogen atom.

20.5 Reactions with Alkanes

Alkanes are generally unreactive toward laboratory acids, bases, oxidizing agents, and reducing agents. They do burn (undergo combustion reactions) and undergo substitution reactions with halogens to create halogenated hydrocarbons.

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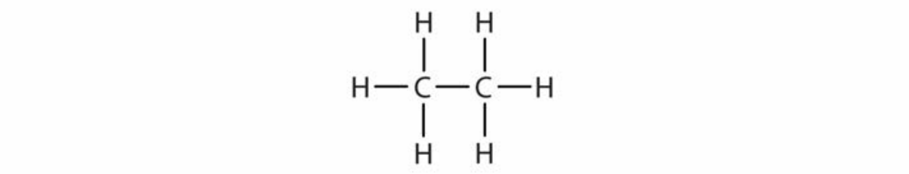
CHAPTER 20 - REVIEW

20.1 Characteristics of Alkanes

1. Without referring to a table, predict which has a higher boiling point—hexane or octane. Explain. **Check answer**[1]
2. If 25 mL of hexane were added to 100 mL of water in a beaker, which of the following would you expect to happen? Explain.
   a. Hexane would dissolve in water.
   b. Hexane would not dissolve in water and would float on top. **Check answer** [2]
   c. Hexane would not dissolve in water and would sink to the bottom of the container.
3. Without referring to a table or other reference, predict which member of each pair has the higher boiling point.
   a. pentane or butane **Check answer**[3]
   b. heptane or nonane **Check answer**[4]
4. For which member of each pair is hexane a good solvent?
   a. pentane or water
   b. sodium chloride or soybean oil
5. Why are alkanes sometimes called paraffins? **Check answer** [5]

20.2 Alkane Formulas

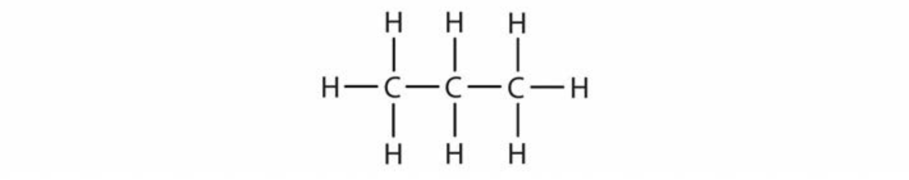
1. Write the condensed structural formula for each structural formula.



(credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

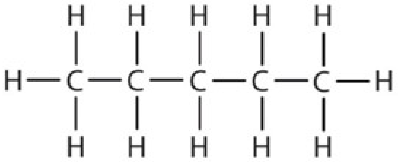
   a. **Check answer**[6]

   b.



(credit: *Intro Chem: GOB (V. 1.0).*, CC BY-NC-SA 3.0).

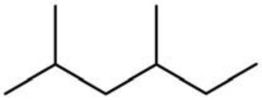
Check answer[7]



(credit: *Intro Chem: GOB (V. 1.0).* , CC BY-NC-SA 3.0).

c. **Check answer**[8]

2. A condensed structural formula for isohexane can be written as $(CH_3)_2CHCH_2CH_2CH_3$. Draw the line-angle formula for isohexane.
3. Draw a line-angle formula for the compound $CH_3CH_2CH(CH_3)CH_2CH_2CH_3$. **Check answer**[9]
4. Give the structural formula for the compound represented by this line-angle formula:



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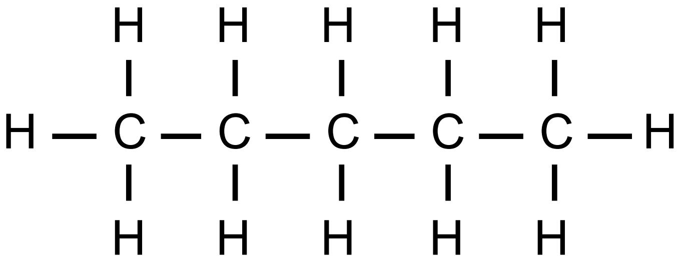
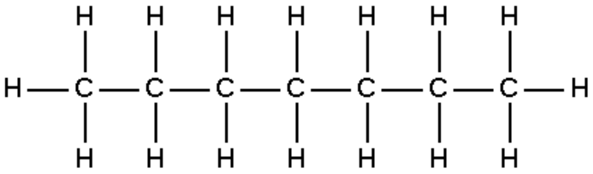
20.3 Isomers of Alkanes and IUPAC Nomenclature

1. Briefly identify the important distinctions between a straight-chain alkane and a branched-chain alkane. **Check answer** [10]
2. How are butane and isobutane related? How do they differ?
3. Name each compound.



(Credit: Photo by Bangin, Public Domain)

   1. **Check answer**[11]
   2. 

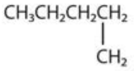
(Credit: Photo by Magnus Manske , Public Domain)

Check answer[12]

4. Write the structural formula for each compound.
    a. hexane
    b. octane

5. Indicate whether the structures in each set represent the same compound or isomers.

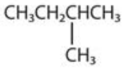
    a. $CH_3CH_2CH_2CH_3$ and



$CH_3CH_2CH_2\underset{\displaystyle CH_2}{\underset{|}{CH_2}}$

Check answer[13](credit: *Intro Chem: GOB (V. 1.0).*, *CC BY-NC-SA 3.0).*

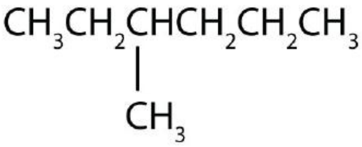
    b. $CH_3CH_2CH_2CH_2CH_3$ and



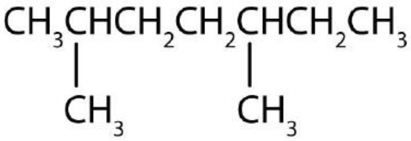
$CH_3CH_2\underset{\displaystyle CH_3}{\underset{|}{C}}HCH_3$

Check answer[14](Credit: *Introduction to Chemistry: General, Organic, and Biological (V. 1.0).* ,CC BY-NC-SA 3.0.)

6. Briefly identify the important distinctions between an alkane and an alkyl group. **Check answer**[15]
7. How many carbon atoms are present in each molecule?
    a. 2-methylbutane
    b. 3-ethylpentane
8. How many carbon atoms are present in each molecule?
    a. 2,3-dimethylbutane **Check answer**[16]
    b. 3-ethyl-2-methylheptane **Check answer** [17]
9. Draw the structure for each compound.
    a. 3-methylpentane
    b. 2,2,5-trimethylhexane
    c. 4-ethyl-3-methyloctane
10. Draw the structure for each compound.
    a. 2-methylpentane **Check answer**[18]
    b. 4-ethyl-2-methylhexane **Check answer**[19]
    c. 2,2,3,3-tetramethylbutane **Check answer** [20]
11. Name each compound according to the IUPAC system.

a. 
$CH_3CH_2\underset{\underset{CH_3}{|}}{C}HCH_2CH_2CH_3$

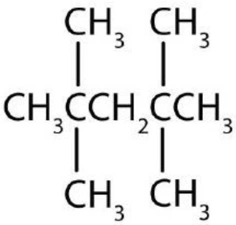
(credit: *Intro Chem: GOB (V. 1.0).* , CC BY-NC-SA 3.0).

b. 
$CH_3\underset{\underset{CH_3}{|}}{C}HCH_2CH_2\underset{\underset{CH_3}{|}}{C}HCH_2CH_3$

(credit: *Intro Chem: GOB (V. 1.0).* , CC BY-NC-SA 3.0).

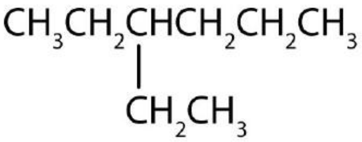
c.

12. Name each compound according to the IUPAC system.


$CH_3\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}CH_2\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}CH_3$

(credit: *Intro Chem: GOB (V. 1.0).* , CC BY-NC-SA 3.0).

a. **Check answer**[21]

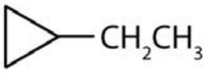
b. 
$CH_3CH_2\underset{\underset{CH_2CH_3}{|}}{C}HCH_2CH_2CH_3$

(credit: *Intro Chem: GOB (V. 1.0).* , CC BY-NC-SA 3.0).

13. What is a substituent? How is the location of a substituent indicated in the IUPAC system?
14. Briefly identify the important distinctions between a common name and an IUPAC name. **Check answer**[22]
15. Draw the structures for the five isomeric hexanes (C_6H_{14}). Name each by the IUPAC system. **Check answer**[23]

20.4 Cycloalkanes

1. What is the molecular formula of cyclooctane? **Check answer**[24]
2. What is the IUPAC name for this compound? **Check answer**[25]



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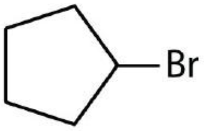
3. Draw the structure for each compound.
   a. ethylcyclobutane **Check answer**[26]
   b. propylcyclopropane **Check answer**[27]
4. Draw the structure for each compound.
   a. methylcyclohexane
   b. butylcyclobutane
5. Cycloalkyl groups can be derived from cycloalkanes in the same way that alkyl groups are derived from alkanes. These groups are named as cyclopropyl, cyclobutyl, and so on. Name each cycloalkyl halide.



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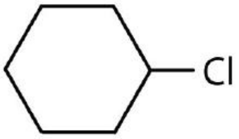
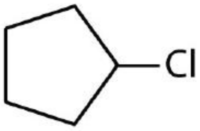
   a. **Check answer**[28]



(credit: *Intro Chem: GOB (V. 1.0).* , CC BY-NC-SA 3.0).

   b. **Check answer**[29]
6. Halogenated cycloalkanes can be named by the IUPAC system. As with alkyl derivatives, monosubstituted derivatives need no number to indicate the position of the halogen. To name disubstituted derivatives, the carbon atoms are numbered starting at the position of one substituent (C1) and proceeding to the second substituted atom by the shortest route. Name each compound.



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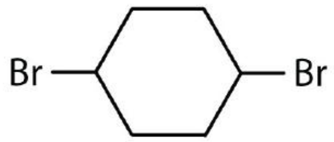
   a.

b. 

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20.5 Halogenated Alkanes

1. What is the IUPAC name for the HFC that has the formula CH_2FCF_3? (Hint: you must use a number to indicate the location of each substituent F atom.) **Check answer** [30]
2. What is the IUPAC name for the HCFC that has the formula $CHCl_2CF_3$? **Check answer**[31]
3. Write the condensed structural formula for each compound.
   a. methyl chloride **Check answer**[32]
   b. chloroform **Check answer**[33]
4. Write the condensed structural formula for each compound.
   a. ethyl bromide
   b. carbon tetrachloride
5. Write the condensed structural formulas for the two isomers that have the molecular formula C_3H_7Br. Give the common name and the IUPAC name of each. **Check answer** [34]
6. Write the condensed structural formulas for the four isomers that have the molecular formula C_4H_9Br. Give the IUPAC name of each.
7. What is a CFC? How are CFCs involved in the destruction of the ozone layer? **Check answer** [35]
8. Explain why each compound is less destructive to the ozone layer than are CFCs.
   a. fluorocarbons
   b. HCFCs

20.6 Reactions of Alkanes

1. Which halogen reacts most readily with alkanes? Which reacts least readily? **Check answer** [36]
2. Why do alkanes usually not react with ionic compounds such as most laboratory acids, bases, oxidizing agents, or reducing agents? **Check answer**[37]
3. Write an equation for the complete combustion of methane (CH_4), the main component of natural gas.
4. What is the most important reaction of alkanes?
5. Name some substances other than oxygen that react readily with alkanes.
6. Write equations for the complete combustion of each compound.
   a. propane (a bottled gas fuel) **Check answer**[38]

b. octane (a typical hydrocarbon in gasoline). **Check answer**[39]

Links to Enhanced Learning

Create your own organic nomenclature quiz to identify, name and draw alkanes using Organic Nomenclature (orgchem101.com). You can customize the types of questions you receive and get instant feedback.

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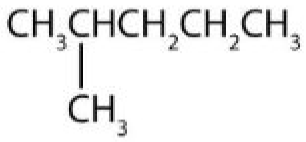
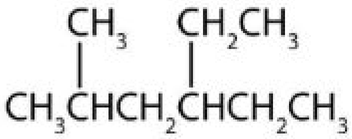
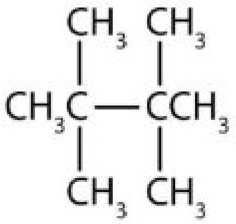
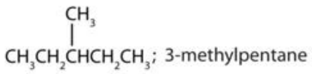
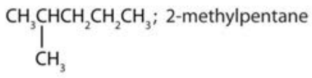
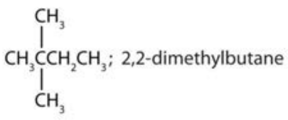
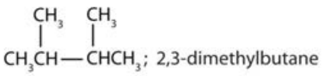
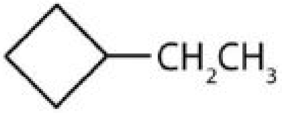
Notes

1. octane because of its greater molar mass
2. b; hexane is insoluble in water and less dense than water.
3. pentane
4. nonane
5. Alkanes do not react with many common chemicals. They are sometimes called paraffins, from the Latin parum affinis, meaning "little affinity."
6. CH_3CH_3
7. $CH_3CH_2CH_3$
8. $CH_3CH_2CH_2CH_2CH_3$
9. 

10. Straight-chain alkanes and branched-chain alkanes have different properties as well as different structures.
11. pentane
12. heptane
13. no
14. yes
15. An alkane is a molecule; an alkyl group is not an independent molecule but rather a part of a molecule that we consider as a unit.
16. 6
17. 10
18. 
$CH_3\underset{\underset{CH_3}{|}}{C}HCH_2CH_2CH_3$
19. 
$CH_3\overset{\overset{CH_3}{|}}{C}HCH_2\overset{\overset{CH_2CH_3}{|}}{C}HCH_2CH_3$
20. 
$CH_3\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}CH_3$
21. 2,2,4,4-tetramethylpentane
22. Common names are widely used but not very systematic; IUPAC names identify a parent compound and name other groups as substituents.
23.
    a. $CH_3CH_2CH_2CH_2CH_2CH_3$; hexane
    b. 
    $CH_3CH_2\overset{\overset{CH_3}{|}}{C}HCH_2CH_3$; 3-methylpentane
    c. 
    $CH_3\underset{\underset{CH_3}{|}}{C}HCH_2CH_2CH_3$; 2-methylpentane
    d. 
    $CH_3\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}CH_2CH_3$; 2,2-dimethylbutane
    e. 
    $CH_3\overset{\overset{CH_3}{|}}{C}H-\overset{\overset{CH_3}{|}}{C}HCH_3$; 2,3-dimethylbutane
    f. C_8H_{16}
    g. ethylcyclopropane

h.



i.

j. cyclopentyl bromide

k. cyclohexyl chloride

l. 1,1,1,2-tetrafluoroethane

m. 1,1,1-trifluoro-2,2-dichloroethane

n. CH_3Cl

o. $CHCl_3$

p. $CH_3CH_2CH_2Br$, propyl bromide, 1-bromopropane; $CH_3CHBrCH_3$, isopropyl bromide, 2-bromopropane

q. compounds containing Cl, F, and C; by releasing Cl atoms in the stratosphere

r. most readily: F_2; least readily: I_2

s. Alkanes are nonpolar; they do not attract ions.

t. $C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$

u. $2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O$

CHAPTER 20 - INFOGRAPHIC DESCRIPTIONS

Infographics used in Chapter 20

- 20.2a A Brief Guide to Types of Organic Chemistry Formulae
- 20.3a A Brief Guide to Types of Isomerism in Organic Chemistry
- 20.3b A Basic Guide to Decoding Organic Compound Names
- 20.6a The Chemistry of Petrol & The Tetraethyl Lead Story
- 20.6b Today in Chemistry History: Susan Solomon, ozone depletion, and CFCs

20.2a A Brief Guide to Types of Organic Chemistry Formulae

Infographic of a guide to formulae in organic chemistry.

- **Molecular formula**: The molecular formula of an organic compound simply shows the number of each type of atom present. It tells you nothing about the bonding within the compound. Example: $C_4H_8O_2$.
- **Empirical formula**: The empirical formula of an organic compound gives the simplest possible whole number ratio of the different types of atoms within the compound. Example: C_2H_4O.
- **Condensed formula**: In condensed formulae, each formulae atom is listed separately, with atoms attached to it following. In cyclic parts of molecules, like benzene, carbons are grouped.
- **Displayed formula**: A displaced formula shows all of the atoms and all of the bonds present in an organic compound. The bonds are represented as lines.
- **Structural formula:** Similar to displayed formula; not all bonds are shown, although all atoms are still indicated using script numbers. Carbon hydrogen bonds are often simplified.
- **Skeletal formula:** In skeletal formulae, most hydrogen atoms are omitted. Line ends or vertices represent carbon. Functional groups and atoms other than carbon or hydrogen are still shown.

Read more about "A Brief Guide to Types of Organic Chemistry Formulae [New tab] *(https://www.compoundchem.com/2014/04/11/a-brief-guide-to-types-of-organic-chemistry-formula/)" by Andy Brunning / Compound Interest, CC BY-NC-ND*

20.3a A Brief Guide to Types of Isomerism in Organic Chemistry

Infographic about the types of isomerism in organic chemistry.

A guide to the five main types of isomerism that can be exhibited by organic compounds. An isomer of a molecule is a molecule with the same molecular formula but a different structural or spatial arrangement of atoms. This variation can lead to a difference in physical or chemical properties.

Structural isomerism:

- **Chain**: different arrangement of molecule's carbon skeleton. The position of the carbon atoms in the molecule can be rearranged to give 'branched' carbon chains coming off the main chain. The name of the molecule changes to reflect this, but the molecular formula is still the same. Examples: Butane, 2-Methyl propane.
- **Position**: The differing position of the same functional group in the molecule. The molecular formula remains the same; the type of functional group also remains the same, but its position in the molecule changes. The name of the molecule changes to reflect the new position of the functional group. Examples: But-2-ene, But-1-ene.
- **Functional**: Differing positions of atoms give a different functional group. Also referred to as functional group isomerism, these isomers have the same molecular formula but the atoms are rearranged to five a different functional group. The name of the molecule changes to reflect the new functional group. Examples: But-2-ene, Cyclobutane.

Stereoisomerism:

- **Geometric**: Different substituents around a bond with restricted rotation. Commonly exhibited by alkenes, the presence of two different substituents on both carbon atoms at wither end of the double bond can give rise to two different, non-superimposable isomers due to the restricted rotation of the bond. Examples: (E)-1,2-Dicholorethene , (Z)-1,2-Dichloroethene.
- **Optical**: Non-superimposable mirror images of the same molecule. Optical isomers differ by the placement of different substituents, around one or more atoms in a molecule. Different arrangements of these substituents can be impossible to superimpose – these are optical isomers.

Read more about "A Brief Guide to Types of Isomerism in Organic Chemistry [New tab] *(https://www.compoundchem.com/2014/05/22/typesofisomerism/)" by Andy Brunning / Compound Interest, CC BY-NC-ND*

20.3b A Basic Guide to Decoding Organic Compound Names

Infographic of basic guide to decoding organic compound names. The names of organic molecules can be long and look lie a confusing mix of words and numbers. However, they follow a particular set of rules which allows their structure to be decoded from their name.

- **Organic compound representation:** Organic molecules are usually represented using skeletal formula. In these diagrams, the line ends and vertices represent carbon atoms. Hydrogen atoms are 'implied' – that is, they are not usually shown, but each carbon must have four bonds, and it's assumed they have the required number of hydrogens for this to be the case. Atoms other than carbon or hydrogen are always shown, and hydrogen atoms are shown if they are bonded to one of these 'heteroatoms'.
- **Functional groups**: A molecule's functional group is the group of atoms that give it its chemical properties and reactivity. It's usually indicated by a suffix at the end of the name, with a number indicating its position if this is required for clarity. There are many different functional groups. Different functional groups have different suffixes. Examples of funcitonal groups: Alchohols (-ol) e.g. ethanol, aldehydes (-al) e.g. ethanal, ketones (-one) e.g. propane, and amine (-amine) e.g. ethanamine.
- **Bond types**: Carbon atoms can be lined by single bonds, double bonds, or even triple bonds. The name of the molecules reflects the bonds present.

Types of molecule bonds

Phrase present in the name	Type of molecule bond present
-an-	molecule contains only single bonds.
-en-	molecule contains at least 1 double bond.
-yn-	molecule contains at least 1 triple bond.
Double or triple bonds	numbers indicate their position.

- **Parent chain:** Part of the organic molecule's name denotes how many carbons make up its 'parent chain'. This is defined as the longest continuously connected chain of carbon atoms including the functional group in the molecule. Carbons not included are dealt with as 'side chains'. Examples: Butane, Hexane.

Number of carbons denoted by prefix

Prefix	Number of carbons
Meth-	1
Eth-	2
Prop-	3
But-	4
Pent-	5
Hex-	6
Hept-	7
Oct-	8
Non-	9
Dec-	10

- **Side chains**: Molecules can have one or more carbons that aren't part of the parent chain, referred to as a 'side chain'. The number of carbons in the side chain is used to name it, in the same way as for the parent chain, but the ending -yl is then added. A number is added to show the location of the side chain on the parent chain. If there is more than one of the same side chain at different points, the prefixes di- (2), tri- (3), or tetra- (4) are used in the name. Examples: 2-Methylbutane, 3-Methylpentane, 2-4-Dimethylpentane, 4-Ethylnonan-1-Ol, 3,5,7-Trimethyldecane.
- **Stereoisomerism**: Chemical names sometimes contain a letter in brackets; for examples, (Z), (E), (R), or (S). These refer to stereoisomerism: when a molecules has the same chemical formula as another, but a different arrangement in 3D space. This can be due to a different arrangement of atoms around a double fond, or when a molecule has two different arrangements of four different groups of atoms around a central carbon which are non-superimposable mirror images.

Read more about "A Basic Guide to Decoding Organic Compound Names [New tab] (https://www.compoundchem.com/2015/08/27/org-comp-names/)" by Andy Brunning / Compound Interest, CC BY-NC-ND

20.6a The Chemistry of Petrol & The Tetraethyl Lead Story

Petrol and diesel are obtained by fractional distillation of crude oil. Diesel is removed from crude oil at a higher boiling point, and contains a larger amount of energy per litre, meaning more miles can be covered with the same volume of fuel. Petrol: 35-200 degree Celsius, 5-12 carbons, and 33,7 megajoules per litre. Diesel: 250-300 degrees Celsius, 10-15 carbons, 36.9 megajoules per litre.

In the engine, a mixture of air and fuels is compressed and burned. Combustion forces the piston down, then the piston pushes back up to expel exhaust gases and the cycle begins again. In diesel engines, the fuel is injected after the air has been compressed before combustion.

Engine knocking happens when the combustion of the fuel doesn't occur in sync with the engine cycle, causing lower engine efficiency and engine damage. Octane ratings measure how well fuel avoids this problem; higher values indicate less knocking. Isooctane and *n*-heptane are refences.

Compounds added to petrol to boost octane rating: Tetraethyl lead, was banned in most countries due to releasing toxic lead fumes. Anti-knocking agents used in unleaded petrol: methyl tertiary-butyl ether (MTBE), ethanol, benzene, and toluene.

Read more about "The Chemistry of Petrol & The Tetraethyl Lead Story [New tab] (https://www.compoundchem.com/2016/05/17/petrol/)" by Andy Brunning / Compound Interest, CC BY-NC-ND

20.6b Today in Chemistry History: Susan Solomon, ozone depletion, and CFCs

Susan Solomon was born in 1956. They provided first direct evidence of chlorine compounds breaking down ozone. Solomon's work confirmed that ozone could react with chlorofluorocarbons on the surface of polar stratospheric clouds. Her work informed the Montreal Protocol, legislation which regulates chemicals that damage the ozone layer.

Ozone and Chlorofluorocarbons: In the stratosphere, CFCs are broken down by UV radiation, releasing highly reactive chlorine radicals. These reacts with and break down ozone molecules. The chlorine radicals are regenerated, so they can go on the to react with thousands of ozone molecules.

Read more about "Today in Chemistry History: Susan Solomon, ozone depletion, and CFCs [New tab] (https://www.compoundchem.com/2018/01/19/solomon-cfcs/)" by Andy Brunning / Compound Interest, CC BY-NC-ND

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