

# Nomenclature of Polyfunctional Organic Compounds

With more than 37 million organic compounds known and several thousand more being created daily, naming them all is a real problem. Part of the problem is due to the sheer complexity of organic structures, but part is also due to the fact that chemical names have more than one purpose. For Chemical Abstracts Service (CAS), which catalogs and indexes the worldwide chemical literature, each compound must have only one correct name. It would be chaos if half the entries for  $\text{CH}_3\text{Br}$  were indexed under “M” for methyl bromide and half under “B” for bromomethane. Furthermore, a CAS name must be strictly systematic so that it can be assigned and interpreted by computers; common names are not allowed.

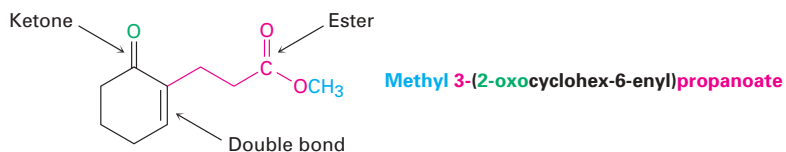
People, however, have different requirements than computers. For people—which is to say chemists in their spoken and written communications—it’s best that a chemical name be pronounceable and that it be as easy as possible to assign and interpret. Furthermore, it’s convenient if names follow historical precedents, even if that means a particularly well-known compound might have more than one name. People can readily understand that bromomethane and methyl bromide both refer to  $\text{CH}_3\text{Br}$ .

As noted in the text, chemists overwhelmingly use the nomenclature system devised and maintained by the International Union of Pure and Applied Chemistry, or IUPAC. Rules for naming monofunctional compounds were given throughout the text as each new functional group was introduced, and a list of where these rules can be found is given in Table A.1.

**Table A.1** Nomenclature Rules for Functional Groups

Functional group	Text section	Functional group	Text section
Acid anhydrides	10.1	Aromatic compounds	5.2
Acid halides	10.1	Carboxylic acids	10.1
Alcohols	8.1	Cycloalkanes	2.7
Aldehydes	9.2	Esters	10.1
Alkanes	2.3	Ethers	8.1
Alkenes	3.1	Ketones	9.2
Alkyl halides	7.1	Nitriles	10.1
Alkynes	3.1	Phenols	8.1
Amides	10.1	Sulfides	8.8
Amines	12.1	Thiols	8.8

Naming a monofunctional compound is reasonably straightforward, but even experienced chemists often encounter problems when faced with naming a complex polyfunctional compound. Take the following compound, for instance. It has three functional groups, ester, ketone, and  $\text{C}=\text{C}$ , but how should it be named? As an ester with an *-oate* ending, a ketone with an *-one* ending, or an alkene with an *-ene* ending? It’s actually named methyl 3-(2-oxocyclohex-6-enyl)propanoate.



The name of a polyfunctional organic molecule has four parts—suffix, parent, prefixes, and locants—which must be identified and expressed in the proper order and format. Let's look at each of the four.

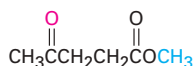
### Name Part 1. The Suffix: Functional-Group Precedence

Although a polyfunctional organic molecule might contain several different functional groups, we must choose just one suffix for nomenclature purposes. It's not correct to use two suffixes. Thus, keto ester **1** must be named either as a ketone with an *-one* suffix or as an ester with an *-oate* suffix, but it can't be named as an *-onoate*. Similarly, amino alcohol **2** must be named either as an alcohol (*-ol*) or as an amine (*-amine*), but it can't be named as an *-olamine* or *-aminol*.

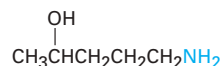


The only exception to the rule requiring a single suffix is when naming compounds that have double or triple bonds. Thus, the unsaturated acid  $\text{H}_2\text{C}=\text{CHCH}_2\text{CO}_2\text{H}$  is but-3-enoic acid, and the acetylenic alcohol  $\text{HC}\equiv\text{CCH}_2\text{CH}_2\text{CH}_2\text{OH}$  is pent-5-yn-1-ol.

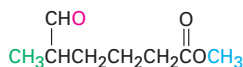
How do we choose which suffix to use? Functional groups are divided into two classes, **principal groups** and **subordinate groups**, as shown in Table A.2. Principal groups can be cited either as prefixes or as suffixes, while subordinate groups are cited only as prefixes. Within the principal groups, an order of priority has been established, with the proper suffix for a given compound determined by choosing the principal group of highest priority. For example, Table A.2 indicates that keto ester **1** should be named as an ester rather than as a ketone because an ester functional group is higher in priority than a ketone. Similarly, amino alcohol **2** should be named as an alcohol rather than as an amine. Thus, the name of **1** is methyl 4-oxopentanoate, and the name of **2** is 5-aminopentan-2-ol. Further examples are shown:



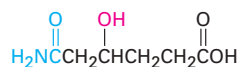
**1. Methyl 4-oxopentanoate**  
(an ester with a ketone group)



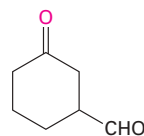
**2. 5-Aminopentan-2-ol**  
(an alcohol with an amine group)



**3. Methyl 5-methyl-6-oxohexanoate**  
(an ester with an aldehyde group)



**4. 5-Carbamoyl-4-hydroxypentanoic acid**  
(a carboxylic acid with amide and alcohol groups)



**5. 3-Oxocyclohexanecarbaldehyde**  
(an aldehyde with a ketone group)

**Table A.2** Classification of Functional Groups<sup>a</sup>

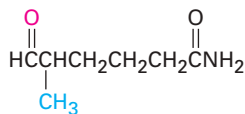
Functional group	Name as suffix	Name as prefix
<b>Principal groups</b>	-oic acid	carboxy
Carboxylic acids	-carboxylic acid	
Acid anhydrides	-oic anhydride -carboxylic anhydride	—
Esters	-oate -carboxylate	alkoxycarbonyl
Thioesters	-thioate -carbothioate	alkylthiocarbonyl
Acid halides	-oyl halide -carbonyl halide	halocarbonyl
Amides	-amide -carboxamide	carbamoyl
Nitriles	-nitrile -carbonitrile	cyano
Aldehydes	-al -carbaldehyde	oxo
Ketones	-one	oxo
Alcohols	-ol	hydroxy
Phenols	-ol	hydroxy
Thiols	-thiol	mercapto
Amines	-amine	amino
Imines	-imine	imino
Ethers	ether	alkoxy
Sulfides	sulfide	alkylthio
Disulfides	disulfide	—
Alkenes	-ene	—
Alkynes	-yne	—
Alkanes	-ane	—
<b>Subordinate groups</b>		
Azides	—	azido
Halides	—	halo
Nitro compounds	—	nitro

<sup>a</sup>Principal groups are listed in order of decreasing priority; subordinate groups have no priority order.

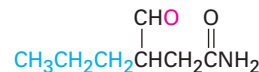
## Name Part 2. The Parent: Selecting the Main Chain or Ring

The parent, or base, name of a polyfunctional organic compound is usually easy to identify. If the principal group of highest priority is part of an open chain, the parent name is that of the longest chain containing the largest number of principal groups. For example, compounds **6** and **7** are isomeric aldehydo amides, which must be named as amides rather than as aldehydes according to Table A.2. The longest chain in compound **6** has six carbons, and the substance is therefore named 5-methyl-6-oxohexanamide. Compound **7** also has a chain of six carbons, but the longest chain that contains both

principal functional groups has only four carbons. The correct name of **7** is 4-oxo-3-propylbutanamide.

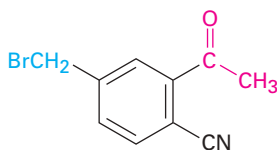


6. 5-Methyl-6-oxohexanamide

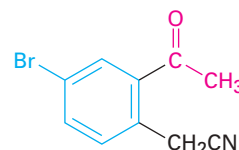


7. 4-Oxo-3-propylbutanamide

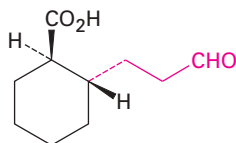
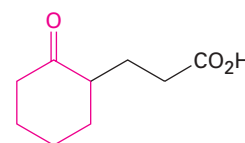
If the highest-priority principal group is attached to a ring, the parent name is that of the ring system. Compounds **8** and **9**, for instance, are isomeric keto nitriles and must both be named as nitriles according to Table A.2. Substance **8** is named as a benzonitrile because the  $-CN$  functional group is a substituent on the aromatic ring, but substance **9** is named as an acetonitrile because the  $-CN$  functional group is on an open chain. The correct names are 2-acetyl-(4-bromomethyl)benzonitrile (**8**) and (2-acetyl-4-bromophenyl)acetonitrile (**9**). As further examples, compounds **10** and **11** are both keto acids and must be named as acids, but the parent name in (**10**) is that of a ring system (cyclohexanecarboxylic acid) and the parent name in (**11**) is that of an open chain (propanoic acid). The full names are *trans*-2-(3-oxopropyl)cyclohexanecarboxylic acid (**10**) and 3-(2-oxocyclohexyl)propanoic acid (**11**).



8. 2-Acetyl-(4-bromomethyl)benzonitrile



9. (2-Acetyl-4-bromophenyl)acetonitrile

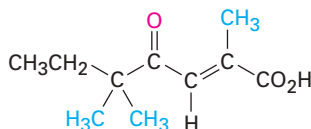
10. *trans*-2-(3-oxopropyl)cyclohexanecarboxylic acid

11. 3-(2-Oxocyclohexyl)propanoic acid

## Name Parts 3 and 4. The Prefixes and Locants

With the parent name and the suffix established, the next step is to identify and give numbers, or *locants*, to all substituents on the parent chain or ring. These substituents include all alkyl groups and all functional groups other than the one cited in the suffix. For example, compound **12** contains three different functional groups (carboxyl, keto, and double bond). Because the carboxyl group is highest in priority and because the longest chain containing the functional groups has seven carbons, **12** is a heptenoic acid. In addition, the main chain has a keto (oxo) substituent and three methyl groups. Numbering from the end nearer the highest-priority functional group, **12** is named (*E*)-2,5,5-trimethyl-4-oxohept-2-enoic acid. Look back at some of the other

compounds we've named to see other examples of how prefixes and locants are assigned.

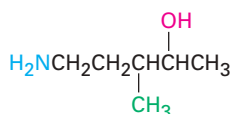


12. (*E*)-2,5,5-Trimethyl-4-oxohept-2-enoic acid

## Writing the Name

Once the name parts have been established, the entire name is written out. Several additional rules apply:

- Order of prefixes.** When the substituents have been identified, the main chain has been numbered, and the proper multipliers such as *di-* and *tri-* have been assigned, the name is written with the substituents listed in alphabetical, rather than numerical, order. Multipliers such as *di-* and *tri-* are not used for alphabetization purposes, but the prefix *iso-* is used.

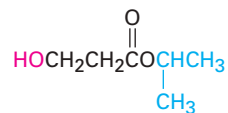


13. 5-Amino-3-methylpentan-2-ol

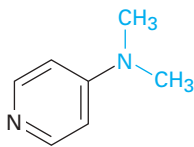
- Use of hyphens; single- and multiple-word names.** The general rule is to determine whether the parent is itself an element or compound. If it is, then the name is written as a single word; if it isn't, then the name is written as multiple words. Methylbenzene is written as one word, for instance, because the parent—benzene—is itself a compound. Diethyl ether, however, is written as two words because the parent—ether—is a class name rather than a compound name. Some further examples follow:



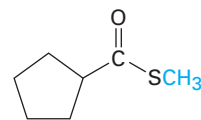
14. **Dimethylmagnesium**  
(one word, because magnesium is an element)



15. **Isopropyl 3-hydroxypropanoate**  
(two words, because "propanoate" is not a compound)

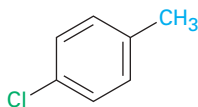
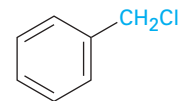
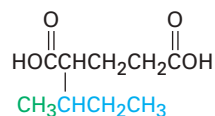


16. **4-(Dimethylamino)pyridine**  
(one word, because pyridine is a compound)



17. **Methyl cyclopentanecarbothioate**  
(two words, because "cyclopentanecarbothioate" is not a compound)

**3. Parentheses.** Parentheses are used to denote complex substituents when ambiguity would otherwise arise. For example, chloromethylbenzene has two substituents on a benzene ring, but (chloromethyl)benzene has only one complex substituent. Note that the expression in parentheses is not set off by hyphens from the rest of the name.

18. **p-Chloromethyl**benzene19. **(Chloromethyl)**benzene20. **2-(1-Methylpropyl)**pentanedioic acid

### Additional Reading

Further explanations of the rules of organic nomenclature can be found online at <http://www.acdlabs.com/iupac/nomenclature/> and in the following references:

1. "A Guide to IUPAC Nomenclature of Organic Compounds," CRC Press, Boca Raton, FL, 1993.
2. "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H," International Union of Pure and Applied Chemistry, Pergamon Press, Oxford, 1979.

# Glossary

**Absorbance** (Section 13.5): In optical spectroscopy, the logarithm of the intensity of the incident light divided by the intensity of the light transmitted through a sample;  $A = \log I_0/I$ .

**Absorption spectrum** (Section 13.2): A plot of wavelength of incident light versus amount of light absorbed. Organic molecules show absorption spectra in both the infrared and ultraviolet regions of the electromagnetic spectrum.

**Acetal** (Section 9.8): A functional group consisting of two  $-OR$  groups bonded to the same carbon,  $R_2C(OR')_2$ . Acetals are often used as protecting groups for ketones and aldehydes.

**Acetyl group** (Section 9.2): The  $CH_3CO-$  group.

**Acetylide anion** (Section 4.11): The anion formed by removal of a proton from a terminal alkyne,  $R-C\equiv C^-$ .

**Achiral** (Section 6.2): Lacking handedness. A molecule is achiral if it has a plane of symmetry and is thus superimposable on its mirror image.

**Acid anhydride** (Section 10.7): A functional group with two acyl groups bonded to a common oxygen atom,  $RCO_2COR'$ .

**Acid halide** (Section 10.7): A functional group with the general formula  $RCOX$ , where  $X$  is a halogen.

**Acidity constant,  $K_a$**  (Section 1.10): A measure of acid strength in water. For any acid  $HA$ , the acidity constant is given by the expression

$$K_a = \frac{[H_3O^+][A^-]}{[HA]}$$

**Activating group** (Section 5.7): An electron-donating group such as hydroxyl ( $-OH$ ) or amino ( $-NH_2$ ) that increases the reactivity of an aromatic ring toward electrophilic aromatic substitution.

**Activation energy,  $E_{act}$**  (Section 3.8): The difference in energy between ground state and transition state. The amount of activation energy required by a reaction determines the rate at which the reaction proceeds.

**Active site** (Section 15.10): The pocket in an enzyme where a substrate is bound and undergoes reaction.

**Acyl group** (Sections 5.5 and 9.2): A name for the  $-COR$  group.

**Acyl phosphate** (Section 10.12): A functional group with an acyl group bonded to a phosphate,  $RCO_2PO_3^{2-}$ .

**Acylation** (Section 5.5): The introduction of an acyl group,  $-COR$ , onto a molecule. For example, acylation of an aromatic ring yields a ketone, acylation of an alcohol yields an ester, and acylation of an amine yields an amide.

**Acylium ion** (Section 5.5): A resonance-stabilized carbocation in which the positive charge is located at a carbonyl-group carbon,  $R-C^+=O \leftrightarrow R-C\equiv O^+$ . Acylium ions are intermediates in Friedel-Crafts acylation reactions.

**1,2-Addition** (Sections 4.8 and 9.10): The addition of a reactant to the two ends of a double bond.

**1,4-Addition** (Sections 4.8 and 9.10): The addition of a reactant to atoms 1 and 4 of a conjugated diene or conjugated enone.

**Addition reaction** (Section 3.5): The reaction that occurs when two reactants combine to form a single new product with no atoms left over.

**Adrenocortical hormone** (Section 16.4): A steroid hormone secreted by the adrenal glands. There are two types of adrenocortical hormones: mineralocorticoids and glucocorticoids.

**Alcohol** (Chapter 8): A compound with an  $-OH$  group bonded to a saturated,  $sp^3$ -hybridized carbon atom.

**Aldaric acid** (Section 14.7): The dicarboxylic acid that results from oxidation of an aldose.

**Aldehyde** (Section 9.1): A compound containing the  $\text{-CHO}$  functional group.

**Alditol** (Section 14.7): The polyalcohol that results from reduction of the carbonyl group of a monosaccharide.

**Aldol reaction** (Section 11.8): A carbonyl condensation reaction between two ketones or aldehydes leading to a  $\beta$ -hydroxy carbonyl product.

**Aldonic acid** (Section 14.7): The monocarboxylic acid that results from mild oxidation of an aldose.

**Aldose** (Section 14.1): A simple sugar with an aldehyde carbonyl group.

**Alicyclic** (Section 2.7): An aliphatic cyclic hydrocarbon, or cycloalkane.

**Aliphatic** (Section 2.2): A nonaromatic hydrocarbon such as a simple alkane, alkene, or alkyne.

**Alkaloid** (Section 12.7): A naturally occurring compound that contains a basic amine functional group.

**Alkane** (Section 2.2): A compound that contains only carbon and hydrogen and has only single bonds.

**Alkene** (Chapter 3 Introduction): A hydrocarbon that contains a carbon-carbon double bond,  $\text{R}_2\text{C}=\text{CR}_2$ .

**Alkoxide ion** (Section 8.2): The anion  $\text{RO}^-$  formed by deprotonation of an alcohol.

**Alkyl group** (Section 2.2): The partial structure that remains when a hydrogen atom is removed from an alkane.

**Alkyl halide** (Chapter 7 Introduction): A compound with a halogen atom bonded to a saturated,  $\text{sp}^3$ -hybridized carbon atom.

**Alkylamine** (Section 12.1): An amino-substituted alkane,  $\text{RNH}_2$ ,  $\text{R}_2\text{NH}$ , or  $\text{R}_3\text{N}$ .

**Alkylation** (Sections 5.5 and 11.6): The introduction of an alkyl group onto a molecule. For example, aromatic rings can be alkylated to yield arenes ( $\text{ArH} \rightarrow \text{ArR}$ ), and enolate anions can be alkylated to yield  $\alpha$ -substituted carbonyl compounds.

**Alkyne** (Chapter 3 Introduction): A hydrocarbon that has a carbon-carbon triple bond.

**Allylic** (Section 4.8): The position next to a double bond.

**$\alpha$ -Amino acid** (Section 15.1): A compound with an amino group attached to the carbon atom next to the carboxyl group,  $\text{RCH}(\text{NH}_2)\text{CO}_2\text{H}$ .

**$\alpha$  Anomer** (Section 14.6): The cyclic hemiacetal form of a sugar that has the hemiacetal  $\text{-OH}$  group on the side of the ring opposite the terminal  $\text{-CH}_2\text{OH}$ .

**$\alpha$  Helix** (Section 15.8): A common secondary structure of a protein in which the chain coils into a spiral.

**$\alpha$  Position** (Chapter 11 Introduction): The position next to a carbonyl group.

**$\alpha$ -Substitution reaction** (Section 11.2): A reaction that results in substitution of a hydrogen on the  $\alpha$  carbon of a carbonyl compound.

**$\alpha$ ,  $\beta$ -Unsaturated carbonyl compound** (Section 9.10): A compound containing the  $\text{C}=\text{C}-\text{C}=\text{O}$  functional group.

**Amide** (Section 10.10): A compound containing the  $\text{-CONR}_2$  functional group.

**Amine** (Section 12.1): An organic derivative of ammonia,  $\text{RNH}_2$ ,  $\text{R}_2\text{NH}$ , or  $\text{R}_3\text{N}$ .

**Amino acid** (Section 15.1): See  $\alpha$ -Amino acid.

**Amino sugar** (Section 14.8): A sugar with one of its  $\text{-OH}$  groups replaced by  $\text{-NH}_2$ .

**Amphiprotic** (Section 15.1): Capable of acting as either an acid or a base.

**Amplitude** (Section 13.2): The height of a wave from midpoint to peak.

**Anabolism** (Section 17.1): Metabolic reactions that synthesize larger molecules from smaller precursors.

**Androgen** (Section 16.4): A steroid male sex hormone such as testosterone.

**Angle strain** (Section 2.9): The strain introduced into a molecule when a bond angle is deformed from its ideal value.

**Anomeric center** (Section 14.6): The hemiacetal carbon atom in the cyclic pyranose or furanose form of a sugar.

**Anomers** (Section 14.6): Cyclic stereoisomers of sugars that differ only in their configurations at the hemiacetal (anomeric) carbon.



**Anti stereochemistry** (Section 4.4): The opposite of syn. An anti addition reaction is one in which the two ends of the double bond are attacked from different sides.

**Anticodon** (Section 16.9): A sequence of three bases on tRNA that read the codons on mRNA and bring the correct amino acids into position for protein synthesis.

**Antisense strand** (Section 16.8): The noncoding strand of double-helical DNA that does not contain the gene.

**Aromatic** (Section 5.1): The class of compounds that contain a benzene-like six-membered ring with three double bonds.

**Aryl group** (Section 5.2): An aromatic substituent group, Ar<sup>-</sup>.

**Arylamine** (Section 12.1): An amino-substituted aromatic compound, ArNH<sub>2</sub>.

**Axial position** (Section 2.10): A bond to chair cyclohexane that lies along the ring axis perpendicular to the rough plane of the ring.

**Backbone** (Section 15.3): The repeating series of -N-CH-CO- atoms that make up a protein chain.

**Base peak** (Section 13.1): The most intense peak in a mass spectrum.

**Basicity constant,  $K_b$**  (Section 12.3): A value that expresses the strength of a base in water solution. The larger the  $K_b$ , the stronger the base.

**Benzoyl group** (Section 9.2): The C<sub>6</sub>H<sub>5</sub>CO- group.

**Benzyl group** (Section 5.2): The C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>- group.

**Benzylic position** (Section 5.8): The position next to an aromatic ring.

**$\beta$  Anomer** (Section 14.6): The cyclic hemiacetal form of a sugar that has the hemiacetal -OH group on the same side of the ring as the terminal -CH<sub>2</sub>OH.

**$\beta$ -Oxidation pathway** (Section 17.2): A series of four enzyme-catalyzed reactions that cleave two carbon atoms at a time from the end of a fatty-acid chain.

**$\beta$ -Pleated sheet** (Section 15.8): A protein secondary structure in which the chain folds back on itself so that two sections of the chain run parallel.

**Bimolecular reaction** (Section 7.5): A reaction whose rate-limiting step occurs between two reactants.

**Boc derivative** (Section 15.7): A butyloxycarbonyl N-protected amino acid.

**Bond angle** (Section 1.6): The angle formed between two adjacent bonds.

**Bond length** (Section 1.5): The equilibrium distance between the nuclei of two atoms that are bonded to each other.

**Bond strength** (Section 1.5): The amount of energy needed to break a bond to produce two radical fragments.

**Branched-chain alkane** (Section 2.2): An alkane that contains a branching connection of carbons as opposed to a straight-chain alkane.

**Bromonium ion** (Section 4.4): A species with a divalent, positively charged bromine, R<sub>2</sub>Br<sup>+</sup>.

**Brønsted-Lowry acid** (Section 1.10): A substance that donates a hydrogen ion (proton, H<sup>+</sup>) to a base.

**Brønsted-Lowry base** (Section 1.10): A substance that accepts a hydrogen ion, H<sup>+</sup>, from an acid.

**C-Terminal amino acid** (Section 15.3): The amino acid with a free -CO<sub>2</sub>H group at one end of a protein chain.

**Cahn-Ingold-Prelog sequence rules** (Sections 3.4 and 6.5): A series of rules for assigning relative rankings to substituent groups on a double-bond carbon atom or on a chirality center.

**Carbanion** (Section 7.3): A carbon-anion, or substance that contains a trivalent, negatively charged carbon atom (R<sub>3</sub>C<sup>-</sup>).

**Carbocation** (Section 3.7): A carbon-cation, or substance that contains a trivalent, positively charged carbon atom having six electrons in its outer shell (R<sub>3</sub>C<sup>+</sup>).

**Carbohydrate** (Section 14.1): A polyhydroxy aldehyde or polyhydroxy ketone. Carbohydrates can be either simple sugars such as glucose or complex sugars such as cellulose.

**Carbonyl condensation reaction** (Section 11.7): A reaction between two carbonyl compounds in which the  $\alpha$  carbon of one partner bonds to the carbonyl carbon of the other.

**Carbonyl group** (Section 9.1): The C=O functional group.

**Carboxyl group** (Section 10.1): The  $-\text{CO}_2\text{H}$  group.

**Carboxylate ion** (Section 10.3): The anion of a carboxylic acid,  $\text{RCO}_2^-$ .

**Carboxylic acid** (Section 10.1): A compound containing the  $-\text{CO}_2\text{H}$  functional group.

**Carboxylic acid derivative** (Chapter 10 Introduction): A compound in which an acyl group is bonded to an electronegative atom or substituent that can act as a leaving group in a substitution reaction. Esters, amides, and acid halides are examples.

**Catabolism** (Section 17.1): Metabolic reactions that break down large molecules.

**Catalyst** (Section 3.9): A substance that increases the rate of a chemical transformation by providing an alternative mechanism but is not itself changed in the reaction.

**Chain-growth polymer** (Section 10.13): A polymer produced by chain reaction of a monofunctional monomer.

**Chair conformation** (Section 2.9): A three-dimensional conformation of cyclohexane that resembles the rough shape of a chair. The chair form of cyclohexane has neither angle strain nor eclipsing strain.

**Chemical shift** (Section 13.9): The position on the NMR chart where a nucleus absorbs. By convention, the chemical shift of tetramethylsilane is set at zero and all other absorptions usually occur downfield (to the left on the chart).

**Chiral** (Section 6.2): Having handedness. A chiral molecule does not have a plane of symmetry, is not superimposable on its mirror image, and thus exists in right- and left-handed forms.

**Chiral environment** (Section 6.10): Chiral surroundings or conditions in which a molecule resides.

**Chirality center** (Section 6.2): An atom (usually carbon) that is bonded to four different groups. Also called a stereocenter.

**Cis-trans isomers** (Sections 2.8 and 3.3): Stereoisomers that differ in their stereochemistry about a double bond or a ring.

**Citric acid cycle** (Section 17.4): The metabolic pathway by which acetyl CoA is degraded to  $\text{CO}_2$ .

**Claisen condensation reaction** (Section 11.10): A carbonyl condensation reaction between two esters leading to formation of a  $\beta$ -keto ester product.

**Coding strand** (Section 16.8): The sense strand of double-helical DNA that contains the gene.

**Codon** (Section 16.9): A three-base sequence on the mRNA chain that encodes the genetic information necessary to cause specific amino acids to be incorporated into proteins.

**Coenzyme** (Section 15.9): A small organic molecule that acts as an enzyme cofactor.

**Cofactor** (Section 15.9): A small, nonprotein part of an enzyme necessary for biological activity.

**Complex carbohydrate** (Section 14.1): A carbohydrate composed of two or more simple sugars linked together by acetal bonds.

**Condensed structure** (Section 2.2): A shorthand way of drawing structures in which C-H and C-C bonds are understood rather than shown explicitly.

**Configuration** (Section 6.5): The three-dimensional arrangement of atoms bonded to a chirality center.

**Conformation** (Section 2.5): The exact three-dimensional shape of a molecule at any given instant, assuming that rotation around single bonds is frozen.

**Conformers** (Section 2.5): Conformational isomers that interconvert by bond rotation.

**Conjugate acid** (Section 1.10): The product that results when a base accepts  $\text{H}^+$ .

**Conjugate (1,4) addition reaction** (Section 9.10): The addition of a nucleophile to the  $\beta$  carbon atom of an  $\alpha,\beta$ -unsaturated carbonyl compound.

**Conjugate base** (Section 1.10): The anion that results from dissociation of an acid.

**Conjugation** (Section 4.8): A series of alternating single and multiple bonds with overlapping  $p$  orbitals.

**Constitutional isomers** (Section 2.2): Isomers such as butane and 2-methylpropane, which have their atoms connected in a different order.

**Coupled reactions** (Section 17.1): Two reactions that share a common intermediate so that the energy released in the favorable step allows the unfavorable step to occur.

**Coupling constant,  $J$**  (Section 13.12): The magnitude of the spin–spin splitting interaction between nuclei whose spins are coupled.

**Covalent bond** (Section 1.4): A bond formed by sharing electrons between two nuclei.

**Cycloalkane** (Section 2.7): An alkane with a ring of carbon atoms.

**D Sugar** (Section 14.3): A sugar whose hydroxyl group at the chirality center farthest from the carbonyl group points to the right when the molecule is drawn in Fischer projection.

**Deactivating group** (Section 5.7): An electron-withdrawing substituent that decreases the reactivity of an aromatic ring toward electrophilic aromatic substitution.

**Decarboxylation** (Section 11.6): The loss of  $\text{CO}_2$ .  $\beta$ -Keto acids decarboxylate readily on heating.

**Dehydration** (Section 8.4): Elimination of water from an alcohol to yield an alkene.

**Dehydrohalogenation** (Section 7.7): Elimination of HX from an alkyl halide to yield an alkene on treatment with a strong base.

**Delta ( $\delta$ ) scale** (Section 13.9): The arbitrary scale used for defining the position of NMR absorptions;  $1 \delta = 1 \text{ ppm}$  of spectrometer frequency.

**Deoxy sugar** (Section 14.8): A sugar with an  $-\text{OH}$  group missing from one carbon.

**Deoxyribonucleic acid (DNA)** (Section 16.5): The biopolymer consisting of deoxyribonucleotide units linked together through phosphate–sugar bonds. Found in the nucleus of cells, DNA contains an organism’s genetic information.

**Deshielding** (Section 13.9): An effect observed in NMR that causes a nucleus to absorb downfield because of a withdrawal of electron density from the nucleus.

**Dextrorotatory** (Section 6.3): An optically active substance that rotates the plane of polarization of plane-polarized light in a right-handed (clockwise) direction.

**Diastereomers** (Section 6.6): Non–mirror-image stereoisomers; diastereomers have the same configuration at one or more chirality centers but differ at other chirality centers.

**1,3-Diaxial interaction** (Section 2.11): The strain energy caused by a steric interaction between axial groups three carbon atoms apart in chair cyclohexane.

**Digestion** (Section 17.1): The first stage of catabolism, in which food molecules are hydrolyzed to yield fatty acids, amino acids, and monosaccharides.

**Disaccharide** (Section 14.9): A complex carbohydrate formed by linking two simple sugars through an acetal bond.

**Disulfide** (Section 8.8): A compound of the general structure  $\text{RSSR}'$ .

**DNA** (Section 16.5): *See* Deoxyribonucleic acid.

**Double bond** (Section 1.8): A covalent bond formed by sharing two pairs of electrons between atoms.

**Double helix** (Section 16.6): The structure of DNA in which two polynucleotide strands coil around each other.

**Doublet** (Section 13.12): A two-line NMR absorption caused by spin–spin splitting when the spin of the nucleus under observation couples with the spin of a neighboring magnetic nucleus.

**Downfield** (Section 13.9): The left-hand portion of the NMR chart.

***E* geometry** (Section 3.4): A term used to describe the stereochemistry of a carbon–carbon double bond in which higher-ranked groups on each carbon are on opposite sides of the double bond.

**E1 reaction** (Section 7.8): A unimolecular elimination reaction in which the substrate spontaneously dissociates to give a carbocation intermediate, which loses a proton in a separate step.

**E1cB reaction** (Section 7.8): A unimolecular elimination reaction in which a proton is first removed to give a carbanion intermediate, which then expels the leaving group in a separate step.

**E2 reaction** (Section 7.7): A bimolecular elimination reaction in which C–H and C–X bond cleavages are simultaneous.

**Eclipsed conformation** (Section 2.5): The geometric arrangement around a carbon–carbon single bond in which the bonds on one carbon are parallel to the bonds on the neighboring carbon as viewed in a Newman projection.

**Edman degradation** (Section 15.6): A method for selectively cleaving the N-terminal amino acid from a peptide.

**Electromagnetic spectrum** (Section 13.2): The range of electromagnetic energy, including infrared, ultraviolet, and visible radiation.

**Electron-dot structure** (Section 1.4): A representation of a molecule showing valence electrons as dots.

**Electron-transport chain** (Section 17.1): The final stage of catabolism, in which ATP is produced.

**Electronegativity** (Section 1.9): The ability of an atom to attract electrons in a covalent bond. Electronegativity generally increases from right to left and from bottom to top of the periodic table.

**Electrophile** (Section 3.6): An “electron-lover,” or substance that accepts an electron pair from a nucleophile in a polar bond-forming reaction.

**Electrophilic addition reaction** (Section 3.7): The addition of an electrophile to an alkene to yield a saturated product.

**Electrophilic aromatic substitution reaction** (Section 5.3): The substitution of an electrophile for a hydrogen atom on an aromatic ring.

**Electrophoresis** (Sections 15.2 and 16.10): A technique for separating charged organic molecules, particularly proteins and amino acids, by placing them in an electric field.

**Electrostatic potential map** (Section 1.9): A molecular representation that uses color to indicate the calculated charge distribution in the molecule.

**Elimination reaction** (Section 3.5): The reaction that occurs when a single reactant splits apart into two products.

**Emden–Meyerhof pathway** (Section 17.3): An alternative name for glycolysis.

**Enantiomers** (Section 6.1): Stereoisomers that have a mirror-image relationship, with opposite configurations at all chirality centers.

**Enantioselective synthesis** (Chapter 6 *Interlude*): A method of synthesis from an achiral precursor that yields only a single enantiomer of a chiral product.

**3'-End** (Section 16.5): The end of a nucleic acid chain that has a free sugar hydroxyl group.

**5'-End** (Section 16.5): The end of a nucleic acid chain that has a phosphoric acid unit.

**Energy diagram** (Section 3.8): A graph depicting the energy changes that occur during a reaction.

**Enol** (Section 11.1): A vinylic alcohol,  $C=C-OH$ .

**Enolate ion** (Sections 9.10 and 11.1): The resonance-stabilized anion of an enol,  $C=C-O^-$ .

**Enone** (Section 11.9): An unsaturated ketone.

**Entgegen (*E*)** (Section 3.4): A term used to describe the stereochemistry of a carbon–carbon double bond in which higher-ranked groups on each carbon are on opposite sides of the double bond.

**Enzyme** (Section 15.9): A biological catalyst. Enzymes are large proteins that catalyze specific biochemical reactions.

**Epoxide** (Section 4.6): A three-membered ring ether functional group.

**Epoxy resin** (Chapter 8 *Interlude*): A polymer prepared by reaction of a bisphenol with epichlorohydrin.

**Equatorial position** (Section 2.10): A bond to cyclohexane that lies along the rough equator of the ring. (*See Axial position.*)

**Essential amino acid** (Section 15.1): An amino acid that must be obtained in the diet.

**Essential monosaccharide** (Section 14.8): One of eight monosaccharides essential for life and obtained in the diet.

**Essential oil** (Chapter 3 *Interlude*): The fragrant mixture of liquids extracted from many plants.

**Ester** (Section 10.9): A compound containing the  $-CO_2R$  functional group.

**Estrogen** (Section 16.4): A female steroid sex hormone.

**Ether** (Section 8.1): A compound with two organic groups bonded to the same oxygen atom,  $R-O-R'$ .

**Exon** (Section 16.8): A section of DNA that contains genetic information.

**Fat** (Section 16.1): A solid triacylglycerol derived from an animal source.

**Fatty acid** (Section 16.1): A long straight-chain carboxylic acid found in fats and oils.

**Fibrous protein** (Section 15.8): A protein that consists of polypeptide chains arranged side by side in long threads.

**Fingerprint region** (Section 13.3): The complex region of the infrared spectrum from  $1500\text{ cm}^{-1}$  to  $400\text{ cm}^{-1}$ .

**Fischer esterification reaction** (Section 10.6): The acid-catalyzed reaction of an alcohol with a carboxylic acid to yield an ester.

**Fischer projection** (Section 14.2): A method for depicting the configuration of a chirality center using crossed lines. Horizontal bonds come out of the plane of the page, and vertical bonds go back into the plane of the page.

**Fishhook arrow** (Section 3.6): A half-headed curved arrow used to show the movement of a single electron in a radical reaction.

**Fmoc derivative** (Section 15.7): A fluorenylmethyloxycarbonyl N-protected amino acid.

**Formyl group** (Section 9.2): A  $-\text{CHO}$  group.

**Frequency,  $\nu$**  (Section 13.2): The number of electromagnetic wave cycles that travel past a fixed point in a given unit of time, usually expressed in reciprocal seconds,  $\text{s}^{-1}$ , or hertz.

**Friedel–Crafts reaction** (Section 5.5): The introduction of an alkyl or acyl group onto an aromatic ring by an electrophilic substitution reaction.

**Functional group** (Section 2.1): An atom or group of atoms that is part of a larger molecule and has a characteristic chemical reactivity.

**Furanose** (Section 14.5): The five-membered ring structure of a simple sugar.

**Geminal** (Section 9.7): Referring to two groups attached to the same carbon atom.

**Globular protein** (Section 15.8): A protein that is coiled into a compact, nearly spherical shape.

**Glycerophospholipid** (Section 16.3): A lipid that contains a glycerol backbone linked to two fatty acids and a phosphoric acid.

**Glycoconjugate** (Section 14.7): A molecule in which a carbohydrate is linked through its anomeric center to another biological molecule such as a lipid or protein.

**Glycol** (Section 4.6): A diol, such as ethylene glycol,  $\text{HOCH}_2\text{CH}_2\text{OH}$ .

**Glycolipid** (Section 14.7): A biological molecule in which a carbohydrate is linked through its anomeric center to a lipid.

**Glycolysis** (Section 17.3): A series of ten enzyme-catalyzed reactions that break down a glucose molecule into two pyruvate molecules.

**Glycoprotein** (Section 14.7): A biological molecule in which a carbohydrate is linked through its anomeric center to a protein.

**Glycoside** (Section 14.7): A cyclic acetal formed by reaction of a sugar with another alcohol.

**Green chemistry** (Chapter 12 *Interlude*): The design and implementation of chemical products and processes that reduce waste and attempt to eliminate the generation of hazardous substances.

**Grignard reagent** (Section 7.3): An organomagnesium halide,  $\text{RMgX}$ .

**Ground-state electron configuration** (Section 1.2): The lowest-energy electron configuration of a molecule or atom.

**Halogenation** (Sections 4.4 and 5.3): The reaction of halogen with an alkene to yield a 1,2-dihalide addition product or with an aromatic compound to yield a substitution product.

**Hemiacetal** (Section 9.8): A functional group consisting of one  $-\text{OR}$  and one  $-\text{OH}$  group bonded to the same carbon.

**Hertz (Hz)** (Section 13.2): The standard unit for frequency; the number of waves that pass by a fixed point per second.

**Heterocycle** (Sections 5.9 and 12.6): A cyclic molecule whose ring contains more than one kind of atom.

**Hormone** (Section 16.4): A chemical messenger secreted by a specific gland and carried through the bloodstream to affect a target tissue.



**Hybrid orbital** (Section 1.6): An orbital derived from a combination of atomic orbitals. Hybrid orbitals, such as the  $sp^3$ ,  $sp^2$ , and  $sp$  hybrids of carbon, are strongly directed and form stronger bonds than atomic orbitals do.

**Hydration** (Section 4.3): Addition of water to a molecule, such as occurs when alkenes are treated with strong aqueous acid.

**Hydrocarbon** (Section 2.2): A compound that has only carbon and hydrogen.

**Hydrogen bond** (Section 8.2): An attraction between a hydrogen atom bonded to an electronegative element and an electron lone pair on another atom.

**Hydrogenation** (Section 4.5): Addition of hydrogen to a double or triple bond to yield a saturated product.

**Hydrophilic** (Section 16.2): Water-loving; attracted to water.

**Hydrophobic** (Section 16.2): Water-fearing; not attracted to water.

**Hydroquinone** (Section 8.5): 1,4-dihydroxybenzene.

**Hydroxylation** (Section 4.6): The addition of one or more  $-OH$  groups to a molecule.

**Imine** (Section 9.9): A compound with a  $R_2C=NR$  functional group; also called a Schiff base in biochemistry.

**Inductive effect** (Section 1.9): The electron-attracting or electron-withdrawing effect that is transmitted through  $\alpha$  bonds.

**Infrared (IR) spectroscopy** (Section 13.3): A kind of optical spectroscopy that uses infrared energy. IR spectroscopy is particularly useful in organic chemistry for determining the kinds of functional groups in molecules.

**Integration** (Section 13.11): A means of electronically measuring the ratios of the number of nuclei responsible for each peak in an NMR spectrum.

**Intermediate** (Section 3.8): A species that is formed during the course of a multistep reaction but is not the final product.

**Intron** (Section 16.8): A section of DNA that does not contain genetic information.

**Ionic bond** (Section 1.4): A bond between two ions due to the electrical attraction of unlike charges.

**Isoelectric point,  $pI$**  (Section 15.2): The pH at which the number of positive charges and the number of negative charges on a protein or amino acid are exactly balanced.

**Isomers** (Section 2.2): Compounds with the same molecular formula but different structures.

**Isotopes** (Section 1.1): Atoms of the same element that have different mass numbers.

**IUPAC system of nomenclature** (Section 2.3): Rules for naming compounds, devised by the International Union of Pure and Applied Chemistry.

**Kekulé structure** (Section 1.4): A representation of a molecule in which a line between atoms represents a covalent bond.

**Keto-enol tautomerism** (Section 11.1): The equilibration between a carbonyl form and vinylic alcohol form of a molecule.

**Ketone** (Section 9.1): A compound with two organic substituents bonded to a carbonyl group,  $R_2C=O$ .

**Ketose** (Section 14.1): A simple sugar with a ketone functional group.

**Krebs cycle** (Section 17.4): An alternative name for the citric acid cycle, by which acetyl CoA is degraded to  $CO_2$ .

**L Sugar** (Section 14.3): A sugar whose hydroxyl group at the chirality center farthest from the carbonyl group points to the left when the molecule is drawn in Fischer projection.

**Lactam** (Chapter 10 *Interlude*): A cyclic amide.

**$LD_{50}$**  (Chapter 1 *Interlude*): The amount of a substance per kilogram body weight that is lethal to 50% of test animals.

**Leaving group** (Section 7.4): The group that is replaced in a substitution reaction.

**Levorotatory** (Section 6.3): An optically active substance that rotates the plane of polarization of plane-polarized light in a left-handed (counterclockwise) direction.

**Lewis acid** (Section 1.12): A substance with a vacant low-energy orbital that can accept an electron pair from a base.

**Lewis base** (Section 1.12): A substance that donates an electron lone pair to an acid.

**Lewis structure** (Section 1.4): A representation of a molecule showing covalent bonds as a pair of electron dots between atoms.

**Lindlar catalyst** (Section 4.11): A hydrogenation catalyst used to convert an alkyne to a cis alkene.

**Line-bond structure** (Section 1.4): A representation of a molecule showing covalent bonds as lines between atoms.

**1→4 Link** (Section 14.9): An acetal link between the C1 carbonyl group of one sugar and the C4 hydroxyl group of another sugar.

**Lipid** (Chapter 16 Introduction): A naturally occurring substance isolated from plants or animals by extraction with a nonpolar organic solvent.

**Lipid bilayer** (Section 16.3): The double layer of phospholipids that forms a cell membrane.

**Locant** (Sections 2.3 and 3.1): A number in the IUPAC name of a compound that specifies the point of attachment of a substituent to the parent chain or the position of a functional group in the chain.

**Lone-pair electrons** (Section 1.4): A nonbonding electron pair that occupies a valence orbital.

**Magnetic resonance imaging, MRI** (Chapter 13 *Interlude*): A medical diagnostic technique based on nuclear magnetic resonance.

**Major groove** (Section 16.6): The larger of two grooves in double-helical DNA.

**Malonic ester synthesis** (Section 11.6): The synthesis of a carboxylic acid by alkylation of an alkyl halide, followed by hydrolysis and decarboxylation.

**Markovnikov's rule** (Section 4.1): A guide for determining the regiochemistry (orientation) of electrophilic addition reactions. In the addition of HX to an alkene, the hydrogen atom bonds to the alkene carbon that has fewer alkyl substituents.

**Mass spectrometry** (Section 13.1): A technique for measuring the mass, and therefore the molecular weight (MW), of ions.

**Mechanism** (Section 3.6): A complete description of how a reaction occurs. A mechanism accounts for all reactants and all products and describes the details of each individual step in the overall reaction process.

**Mercapto group** (Section 8.8): An alternative name for the thiol group,  $-\text{SH}$ .

**Meso compound** (Section 6.7): A compound that contains one or more chirality centers but is nevertheless achiral because it has a symmetry plane.

**Messenger RNA (mRNA)** (Section 16.8): The kind of RNA transcribed from DNA and used to carry genetic messages from DNA to ribosomes.

**Meta, *m*-** (Section 5.2): A naming prefix used for 1,3-disubstituted benzenes.

**Metabolism** (Section 17.1): A collective name for the many reactions that go on in the cells of living organisms.

**Micelle** (Section 16.2): A spherical cluster of soap-like molecules that aggregate in aqueous solution. The ionic heads of the molecules lie on the outside where they are solvated by water, and the organic tails bunch together on the inside of the micelle.

**Minor groove** (Section 16.6): The smaller groove in double-helical DNA.

**Molar absorptivity** (Section 13.5): A quantitative measure of the amount of UV light absorbed by a sample.

**Molecular ion** (Section 13.1): The cation produced in the mass spectrometer by loss of an electron from the parent molecule. The mass of the molecular ion corresponds to the molecular weight of the sample.

**Molecule** (Section 1.4): A neutral collection of atoms held together by covalent bonds.

**Monomer** (Sections 4.7 and 10.13): The starting unit from which a polymer is made.

**Monosaccharide** (Section 14.1): A simple sugar.

**Monoterpene** (Chapter 3 *Interlude*): A ten-carbon lipid.

**Multiplet** (Section 13.12): A pattern of peaks in an NMR spectrum that arises by spin-spin splitting of a single absorption because of coupling between neighboring magnetic nuclei.

**Mutarotation** (Section 14.6): The change in optical rotation observed when a pure anomer of a sugar is dissolved in water and equilibrates to an equilibrium mixture of anomers.

**$n + 1$  rule** (Section 13.12): The signal of a proton with  $n$  neighboring protons splits into  $n + 1$  peaks in the NMR spectrum.

**N-Terminal amino acid** (Section 15.3): The amino acid with a free  $-\text{NH}_2$  group at one end of a protein chain.

**Natural gas** (Section 2.4): A naturally occurring hydrocarbon mixture consisting chiefly of methane, along with smaller amounts of ethane, propane, and butane.

**Natural product** (Chapter 2 *Interlude*): A catchall term generally taken to mean a small molecule found in bacteria, plants, and other living organisms.

**New molecular entity, NME** (Chapter 2 *Interlude*): A new biologically active chemical substance approved for sale as a drug by the U.S. Food and Drug Administration.

**Newman projection** (Section 2.5): A means of indicating stereochemical relationships between substituent groups on neighboring carbons by looking end-on at a carbon-carbon bond.

**Nitration** (Section 5.4): The substitution of a nitro group onto an aromatic ring.

**Nitrile** (Section 10.11): A compound with a  $-\text{C}\equiv\text{N}$  functional group.

**Node** (Section 1.1): A surface of zero electron density within an orbital. For example, a  $p$  orbital has a nodal plane passing through the center of the nucleus, perpendicular to the axis of the orbital.

**Nonbonding electron** (Section 1.4): A valence electron not used for bonding.

**Nonessential amino acid** (Section 15.1): One of the eleven amino acids that are biosynthesized by humans.

**Normal ( $n$ ) alkane** (Section 2.2): A straight-chain alkane, as opposed to a branched alkane.

**NSAID** (Chapter 5 *Interlude*): A nonsteroidal anti-inflammatory drug, such as aspirin or ibuprofen.

**Nuclear magnetic resonance (NMR) spectroscopy** (Section 13.7): A spectroscopic technique that provides information about the carbon-hydrogen framework of a molecule.

**Nucleic acid** (Section 16.5): A biopolymer, either DNA or RNA, made of nucleotides joined together.

**Nucleophile** (Section 3.6): An electron-rich species that donates an electron pair to an electrophile in a polar bond-forming reaction. Nucleophiles are also Lewis bases.

**Nucleophilic acyl substitution reaction** (Section 10.5): A reaction in which a nucleophile attacks a carbonyl compound and substitutes for a leaving group bonded to the carbonyl carbon.

**Nucleophilic addition reaction** (Section 9.5): A reaction in which a nucleophile adds to the electrophilic carbonyl group of a ketone or aldehyde to give an alcohol.

**Nucleophilic substitution reaction** (Section 7.4): A reaction in which one nucleophile replaces another attached to a saturated carbon atom.

**Nucleoside** (Section 16.5): A nucleic acid constituent, consisting of a sugar residue bonded to a heterocyclic purine or pyrimidine base.

**Nucleotide** (Section 16.5): A nucleic acid constituent, consisting of a sugar residue bonded both to a heterocyclic purine or pyrimidine base and to phosphoric acid.

**Nylon** (Section 10.13): A polyamide step-growth polymer, usually prepared by reaction between a diacid and a diamine.

**Olefin** (Chapter 3 Introduction): An alternative name for an alkene.

**Optical activity** (Section 6.3): The ability of a chiral molecule in solution to rotate plane-polarized light.

**Optical isomers** (Section 6.4): An older, alternative name for enantiomers. Optical isomers are isomers that have a mirror-image relationship.

**Orbital** (Section 1.1): A region of space occupied by a given electron or pair of electrons.

**Organic chemistry** (Chapter 1 Introduction): The chemistry of carbon compounds.

**Organohalide** (Chapter 7 Introduction): A compound that contains one or more halogen atoms bonded to carbon.

**Organometallic compound** (Section 7.3): A compound that contains a carbon-metal bond. Grignard reagents,  $\text{RMgX}$ , are examples.

**Ortho,  $o$ -** (Section 5.2): A naming prefix used for 1,2-disubstituted benzenes.



**Oxidation** (Section 4.6): The addition of oxygen to a molecule or removal of hydrogen from it.

**Oxirane** (Section 4.6): An alternative name for an epoxide.

**Para, *p*-** (Section 5.2): A naming prefix used for 1,4-disubstituted benzenes.

**Paraffin** (Section 2.4): A common name for an alkane.

**Parent peak** (Section 13.1): The peak in a mass spectrum corresponding to the molecular ion and thus representing the molecular weight of the compound.

**Peptide** (Chapter 15 Introduction): A short amino acid polymer in which the individual amino acid residues are linked by amide bonds. (*See* Protein.)

**Peptide bond** (Section 15.4): An amide bond in a peptide chain.

**Peroxyacid** (Section 4.6): A compound with the  $-\text{CO}_3\text{H}$  functional group.

**Petroleum** (Section 2.4): A complex mixture of naturally occurring hydrocarbons derived from the decomposition of plant and animal matter.

**Phenol** (Section 8.1): A compound with an  $-\text{OH}$  group bonded to an aromatic ring,  $\text{ArOH}$ .

**Phenoxide ion** (Section 8.2): The anion of a phenol,  $\text{ArO}^-$ .

**Phenyl group** (Section 5.2): The  $-\text{C}_6\text{H}_5$  group, often abbreviated as  $-\text{Ph}$ .

**Phospholipid** (Section 16.3): A lipid that contains a phosphate residue.

**Phosphoric acid anhydride** (Section 17.1): A substance that contains a  $\text{PO}_2\text{PO}$  link, analogous to the  $\text{CO}_2\text{CO}$  link in carboxylic acid anhydrides.

**Phosphorylation** (Sections 14.7 and 17.1): A reaction that transfers a phosphate group from a phosphoric anhydride to an alcohol.

**Pi ( $\pi$ ) bond** (Section 1.8): A covalent bond formed by sideways overlap of two  $p$  orbitals.

**$\text{p}K_{\text{a}}$**  (Section 1.10): The negative common logarithm of the  $K_{\text{a}}$ ; used to express acid strength.

**Plane of symmetry** (Section 6.2): A plane that bisects a molecule such that one half of the molecule is the mirror image of the other half. Molecules that contain a plane of symmetry are achiral.

**Plane-polarized light** (Section 6.3): Light that has its electric waves oscillating in a single plane rather than in random planes.

**Plasticizer** (Section 10.2): A small organic molecule added to polymers to act as a lubricant between polymer chains.

**Polar covalent bond** (Section 1.9): A covalent bond in which the electrons are shared unequally between the atoms.

**Polar reaction** (Section 3.6): A reaction in which bonds are made when a nucleophile donates two electrons to an electrophile, and in which bonds are broken when one fragment leaves with both electrons from the bond.

**Polarity** (Section 1.9): The unsymmetrical distribution of electrons in a molecule that results when one atom attracts electrons more strongly than another.

**Polycyclic aromatic compound** (Section 5.9): A molecule that has two or more benzene rings fused together.

**Polyester** (Section 10.13): A polymer prepared by reaction between a diacid and a dialcohol.

**Polymer** (Sections 4.7 and 10.13): A large molecule made up of repeating smaller units.

**Polymerase chain reaction (PCR)** (Section 16.11): A method for amplifying small amounts of DNA to prepare larger amounts.

**Polysaccharide** (Section 14.10): A complex carbohydrate that has many simple sugars bonded together by acetal links.

**Polyunsaturated fatty acid** (Section 16.1): A fatty acid with more than one double bond in its chain.

**Primary, secondary, tertiary, quaternary** (Sections 2.2, 8.1, and 12.1): Terms used to describe the substitution pattern at a specific site. A primary site has one organic substituent attached to it, a secondary site has two organic substituents, a tertiary site has three, and a quaternary site has four.

	Carbon	Carbocation	Hydrogen	Alcohol	Amine
Primary	$\text{RCH}_3$	$\text{RCH}_2^+$	$\text{RCH}_3$	$\text{RCH}_2\text{OH}$	$\text{RNH}_2$
Secondary	$\text{R}_2\text{CH}_2$	$\text{R}_2\text{CH}^+$	$\text{R}_2\text{CH}_2$	$\text{R}_2\text{CHOH}$	$\text{R}_2\text{NH}$
Tertiary	$\text{R}_3\text{CH}$	$\text{R}_3\text{C}^+$	$\text{R}_3\text{CH}$	$\text{R}_3\text{COH}$	$\text{R}_3\text{N}$
Quaternary	$\text{R}_4\text{C}$				

**Primary structure** (Section 15.8): The amino acid sequence of a protein.

**Protecting group** (Section 9.8): A group that is temporarily introduced into a molecule to protect a functional group from reaction elsewhere in the molecule.

**Protein** (Chapter 15 Introduction): A large biological polymer containing 50 or more amino acid residues.

**Protein Data Bank** (Chapter 15 *Interlude*): A worldwide online repository of X-ray and NMR structural data for biological macromolecules. To access the Protein Data Bank, go to <http://www.rcsb.org/pdb/>.

**PTH** (Section 15.6): A phenylthiohydantoin derived from a terminal amino acid during Edman degradation.

**Pyranose** (Section 14.5): The six-membered ring structure of a simple sugar.

**Quartet** (Section 13.12): A set of four peaks in an NMR spectrum, caused by spin–spin splitting of a signal by three adjacent nuclear spins.

**Quaternary**: See Primary.

**Quaternary ammonium salt** (Section 12.1): A compound with four organic substituents attached to a positively charged nitrogen,  $R_4N^+ X^-$ .

**Quaternary structure** (Section 15.8): The highest level of protein structure, involving a specific aggregation of individual proteins into a larger cluster.

**Quinone** (Section 8.5): A cyclohexa-2,5-diene-1,4-dione.

**R configuration** (Section 6.5): The configuration at a chirality center as specified using the Cahn–Ingold–Prelog sequence rules.

**R group** (Section 2.2): A generalized abbreviation for an organic partial structure.

**Racemic mixture** (Section 6.8): A 50:50 mixture of the two enantiomers of a chiral substance.

**Radical** (Section 3.6): A species that has an odd number of electrons, such as the chlorine radical,  $Cl\cdot$ .

**Radical reaction** (Section 3.6): A reaction in which bonds are made by donation of one electron from each of two reagents, and in which bonds are broken when each fragment leaves with one electron.

**Reaction intermediate** (Section 3.8): A substance formed transiently during the course of a multistep reaction.

**Reaction mechanism** (Section 3.6): A complete description of how a reaction occurs.

**Rearrangement reaction** (Section 3.5): The reaction that occurs when a single reactant undergoes a reorganization of bonds and atoms to give an isomeric product.

**Reducing sugar** (Section 14.7): A sugar that reduces  $Ag^+$  in the Tollens test or  $Cu^{2+}$  in the Fehling or Benedict tests.

**Reduction** (Section 4.5): The addition of hydrogen to a molecule or the removal of oxygen from it.

**Reductive amination** (Section 12.4): A method for synthesizing amines by treatment of an aldehyde or ketone with ammonia or an amine and a reducing agent.

**Refining** (Section 2.4): The process by which petroleum is converted into gasoline and other useful products.

**Regiospecific** (Section 4.1): A term describing a reaction that occurs with a specific orientation to give a single product rather than a mixture of products.

**Replication** (Section 16.7): The process by which double-stranded DNA uncoils and is replicated to produce two new copies.

**Replication fork** (Section 16.7): The point of unraveling in a DNA chain where replication occurs.

**Residue** (Section 15.3): An amino acid in a protein chain.

**Resolution** (Section 6.8): Separation of a racemic mixture into its pure component enantiomers.

**Resonance forms** (Section 4.9): Structural representations of a molecule that differ only in where the bonding electrons are placed.

**Resonance hybrid** (Section 4.9): The composite structure of a molecule described by different resonance forms.

**Restriction endonuclease** (Section 16.10): An enzyme that is able to cut a DNA strand at a specific base sequence in the chain.

**Ribonucleic acid (RNA)** (Sections 16.5 and 16.8): The biopolymer found in cells that serves to transcribe the genetic information found in DNA and uses that information to direct the synthesis of proteins.

**Ribosomal RNA (rRNA)** (Section 16.8): A kind of RNA that makes up ribosomes.

**Ring-flip** (Section 2.11): The molecular motion that converts one chair conformation of cyclohexane into another chair conformation, thereby interconverting axial and equatorial bonds.

**RNA** (Sections 16.5 and 16.8): *See* Ribonucleic acid.

**S configuration** (Section 6.5): The configuration at a chirality center as specified using the Cahn–Ingold–Prelog sequence rules.

**Saccharide** (Section 14.1): A sugar.

**Salt bridge** (Section 15.8): The ionic attraction between charged amino acid side chains that helps stabilize a protein's tertiary structure.

**Sanger dideoxy method** (Section 16.10): A method for sequencing DNA strands.

**Saponification** (Section 10.9): An old term for the base-induced hydrolysis of an ester to yield a carboxylic acid salt.

**Saturated** (Section 2.2): A compound that has only single bonds.

**Sawhorse representation** (Section 2.5): A manner of representing stereochemistry that uses a stick drawing and gives an oblique view of the conformation around a single bond.

**Schiff base** (Section 17.5): An alternative name for an imine,  $R_2C=NR'$ , used primarily in biochemistry.

**Secondary**: *See* Primary.

**Secondary structure** (Section 15.8): The level of protein substructure that involves organization of chain sections into ordered arrangements such as  $\beta$ -pleated sheets or  $\alpha$  helices.

**Semiconservative replication** (Section 16.7): A description of DNA replication in which each new DNA molecule contains one old strand and one new strand.

**Sense strand** (Section 16.8): The coding strand of double-helical DNA that contains the gene.

**Sequence rules** (Sections 3.4 and 6.5): A series of rules for assigning relative rankings to substituent groups on a double-bond carbon atom or on a chirality center.

**Sesquiterpene** (Chapter 3 *Interlude*): A 15-carbon lipid.

**Shielding** (Section 13.8): An effect observed in NMR that causes a nucleus to absorb toward the right (upfield) side of the chart. Shielding is caused by donation of electron density to the nucleus.

**Side chain** (Section 15.1): The substituent bonded to the  $\alpha$  carbon of an  $\alpha$ -amino acid.

**Sigma ( $\sigma$ ) bond** (Section 1.8): A covalent bond formed by head-on overlap of atomic orbitals.

**Simple sugar** (Section 14.1): A carbohydrate like glucose that can't be hydrolyzed to smaller sugars.

**Skeletal structure** (Section 2.6): A shorthand way of writing structures in which carbon atoms are assumed to be at each intersection of two lines (bonds) and at the end of each line.

**$S_N1$  reaction** (Section 7.6): A nucleophilic substitution reaction that takes place in two steps through a carbocation intermediate.

**$S_N2$  reaction** (Section 7.5): A nucleophilic substitution reaction that takes place in a single step by backside displacement of the leaving group.

**Solid-phase synthesis** (Section 15.7): A technique of synthesis whereby the starting material is covalently bound to a solid polymer bead and reactions are carried out on the bound substrate. After the desired transformations have been effected, the product is cleaved from the polymer.

**$sp$  Hybrid orbital** (Section 1.8): A hybrid orbital derived from the combination of an  $s$  and a  $p$  atomic orbital. The two  $sp$  orbitals that result from hybridization are oriented at an angle of  $180^\circ$  to each other.

**$sp^2$  Hybrid orbital** (Section 1.8): A hybrid orbital derived by combination of an  $s$  atomic orbital with two  $p$  atomic orbitals. The three  $sp^2$  hybrid orbitals that result lie in a plane at angles of  $120^\circ$  to each other.

**$sp^3$  Hybrid orbital** (Section 1.6): A hybrid orbital derived by combination of an  $s$  atomic orbital with three  $p$  atomic orbitals. The four  $sp^3$  hybrid orbitals that result are directed toward the corners of a regular tetrahedron at angles of  $109^\circ$  to each other.

**Specific rotation,  $[\alpha]_D$**  (Section 6.3): The amount by which an optically active compound rotates plane-polarized light under standard conditions.

**Sphingomyelin** (Section 16.3): A phospholipid that has sphingosine as its backbone rather than glycerol.

**Spin–spin splitting** (Section 13.12): The splitting of an NMR signal into a multiplet because of an interaction between nearby magnetic nuclei whose spins are coupled. The magnitude of spin–spin splitting is given by the coupling constant,  $J$ .

**Staggered conformation** (Section 2.5): The three-dimensional arrangement of atoms around a carbon–carbon single bond in which the bonds on one carbon bisect the bond angles on the second carbon as viewed end-on.

**Statins** (Chapter 17 *Interlude*): A drug that blocks the ability of the body to synthesize cholesterol.

**Step-growth polymer** (Section 10.13): A polymer in which each bond is formed independently of the others. Polyesters and polyamides (nylons) are examples.

**Stereocenter** (Section 6.2): An atom in a molecule that is a cause of chirality. Also called a chirality center.

**Stereochemistry** (Sections 2.8 and 6.1): The branch of chemistry concerned with the three-dimensional arrangement of atoms in molecules.

**Stereoisomers** (Section 2.8): Isomers that have their atoms connected in the same order but have different three-dimensional arrangements. The term includes both enantiomers and diastereomers.

**Steric strain** (Section 2.11): The strain imposed on a molecule when two groups are too close together and try to occupy the same space.

**Steroid** (Section 16.4): A lipid whose structure is based on a characteristic tetracyclic carbon skeleton with three 6-membered and one 5-membered ring.

**STR loci** (Chapter 16 *Interlude*): Short tandem repeat sequences of noncoding DNA that are unique to every individual and allow DNA fingerprinting.

**Straight-chain alkane** (Section 2.2): An alkane whose carbon atoms are connected without branching.

**Substitution reaction** (Section 3.5): The reaction that occurs when two reactants exchange parts to give two products.

**Sulfide** (Section 8.8): A compound that has two organic groups bonded to the same sulfur atom,  $R-S-R'$ .

**Symmetry plane** (Section 6.2): A plane that bisects a molecule such that one half of the molecule is the mirror image of the other half. Molecules containing a plane of symmetry are achiral.

**Syn stereochemistry** (Section 4.5): The opposite of anti. A syn addition reaction is one in which the two ends of the double bond react from the same side.

**Tautomers** (Section 11.1): Isomers that interconvert spontaneously, usually with the change in position of a hydrogen.

**Terpenoid** (Chapter 3 *Interlude*): A lipid that is formally derived by head-to-tail polymerization of isoprene units.

**Tertiary**: See Primary.

**Tertiary structure** (Section 15.8): The level of protein structure that involves the manner in which the entire protein chain is folded into a specific three-dimensional arrangement.

**Thioester** (Section 10.12): The sulfur analog of an ester,  $RCOSR'$ .

**Thiol** (Section 8.8): A compound with the  $-SH$  functional group.

**Thiolate ion** (Section 8.8): The sulfur analog of an alkoxide ion,  $RS^-$ .

**Thiophenol** (Chapter 8 Introduction): The sulfur analog of a phenol,  $Ar-SH$ .

**TMS** (Section 13.9): Tetramethylsilane, used as an NMR calibration standard.

**Transamination** (Section 17.5): A reaction in which the  $-NH_2$  group of an amine changes places with the keto group of an  $\alpha$ -keto acid.

**Transcription** (Section 16.8): The process by which the genetic information encoded in DNA is read and used to synthesize RNA in the nucleus of the cell.

**Transfer RNA (tRNA)** (Section 16.8): A kind of RNA that transports amino acids to the ribosomes, where they are joined together to make proteins.

**Transition state** (Section 3.8): An activated complex between reactants, representing the highest energy point on a reaction curve.

**Translation** (Section 16.9): The process by which the genetic information transcribed from DNA onto mRNA is read by tRNA and used to direct protein synthesis.

**Triacylglycerol** (Section 16.1): A lipid, such as that found in animal fat and vegetable oil, that is a triester of glycerol with long-chain fatty acids.

**Tricarboxylic acid cycle** (Section 17.4): An alternative name for the citric acid cycle by which acetyl CoA is degraded to CO<sub>2</sub>.

**Triple bond** (Section 1.8): A covalent bond formed by sharing three pairs of electrons between atoms.

**Triplet** (Section 13.12): A symmetrical three-line splitting pattern observed in the <sup>1</sup>H NMR spectrum when a proton has two equivalent neighbor protons.

**Ultraviolet (UV) spectroscopy** (Section 13.5): An optical spectroscopy employing ultraviolet irradiation. UV spectroscopy provides structural information about the extent of electron conjugation in organic molecules.

**Unimolecular reaction** (Section 7.6): A reaction step that involves only one molecule.

**Unsaturated** (Section 3.1): A molecule that has one or more double or triple bonds and thus has fewer hydrogens than the corresponding alkane.

**Upfield** (Section 13.9): The right-hand portion of the NMR chart.

**Uronic acid** (Section 14.7): The monocarboxylic acid formed by oxidizing the -CH<sub>2</sub>OH end of a sugar without affecting the -CHO end.

**Valence bond theory** (Section 1.5): A theory of chemical bonding that describes bonds as resulting from overlap of atomic orbitals.

**Valence shell** (Section 1.4): The outermost electron shell of an atom.

**Vegetable oil** (Section 16.1): A liquid triacylglycerol derived from a plant source.

**Vinyl monomer** (Section 4.7): A substituted alkene monomer used to make a chain-growth polymer.

**Vinylic** (Section 4.11): Referring to a substituent directly attached to a double-bond carbon atom.

**Vitamin** (Section 15.9): A small organic molecule that must be obtained in the diet and that is required for proper growth.

**Vulcanization** (Chapter 4 *Interlude*): A technique for cross-linking and hardening a diene polymer by heating with a few percent by weight of sulfur.

**Wave equation** (Section 1.1): A mathematical expression that defines the behavior of an electron in an atom.

**Wave function** (Section 1.1): A solution to the wave equation for defining the behavior of an electron in an atom. The square of the wave function defines the shape of an orbital.

**Wavelength,  $\lambda$**  (Section 13.2): The length of a wave from peak to peak.

**Wavenumber,  $\tilde{\nu}$**  (Section 13.2): A unit of frequency measurement equal to the reciprocal of the wavelength in centimeters, cm<sup>-1</sup>.

**Wax** (Section 16.1): A mixture of esters of long-chain carboxylic acids with long-chain alcohols.

**Williamson ether synthesis** (Section 8.4): The reaction of an alkoxide ion with an alkyl halide to yield an ether.

**X-ray crystallography** (Chapter 15 *Interlude*): A technique using X rays to determine the structure of molecules.

**Z geometry** (Section 3.4): A term used to describe the stereochemistry of a carbon-carbon double bond in which the two higher-ranked groups on each carbon are on the same side of the double bond.

**Zaitsev's rule** (Section 7.7): A rule stating that E2 elimination reactions normally yield the more highly substituted alkene as major product.

**Zusammen (Z)** (Section 3.4): A term used to describe the stereochemistry of a carbon-carbon double bond in which the two higher-ranked groups on each carbon are on the same side of the double bond.

**Zwitterion** (Sections 1.11 and 15.1): A neutral dipolar molecule whose positive and negative charges are not adjacent. For example, amino acids exist as zwitterions, H<sub>3</sub>N<sup>+</sup>-CHR-CO<sub>2</sub><sup>-</sup>.

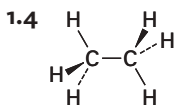
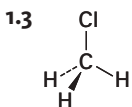
# Answers to Selected In-Chapter Problems

The following answers to in-chapter problems are meant only as a quick check. Full answers and explanations for all problems, both in-chapter and end-of-chapter, are provided in the accompanying *Study Guide and Solutions Manual*.

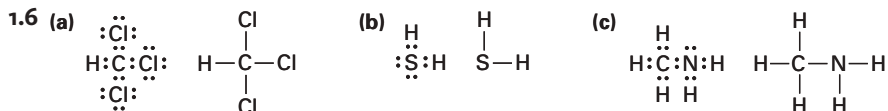
## Chapter 1

1.1 (a) 1 (b) 2 (c) 3

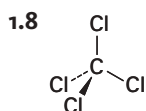
1.2 (a) B:  $1s^2 2s^2 2p$  (b) P:  $1s^2 2s^2 2p^6 3s^2 3p^3$   
 (c) O:  $1s^2 2s^2 2p^4$  (d) Ar:  $1s^2 2s^2 2p^6 3s^2 3p^6$



1.5 (a)  $\text{CCl}_4$  (b)  $\text{AlH}_3$  (c)  $\text{CH}_2\text{Cl}_2$  (d)  $\text{SiF}_4$

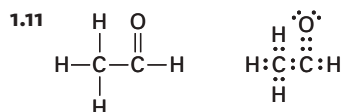
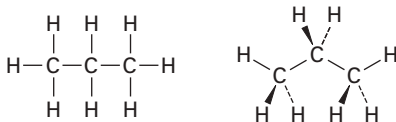


1.7  $\text{C}_2\text{H}_7$  has too many hydrogens for a compound with two carbons.



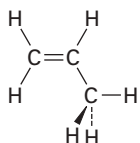
1.9 A carbon atom is larger than a hydrogen atom.

1.10 All bond angles are approximately  $109^\circ$ .



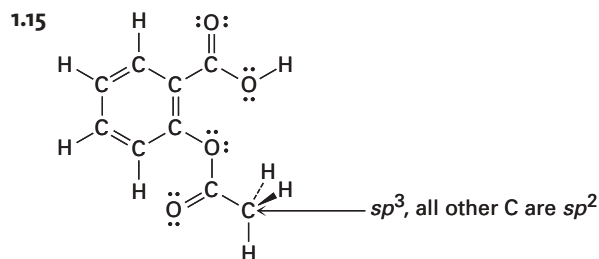


- 1.12 The  $\text{CH}_3$  carbon is  $sp^3$ , the double-bond carbons are  $sp^2$ , and the  $\text{C}=\text{C}-\text{C}$  bond angle is approximately  $120^\circ$ .



- 1.13 The  $\text{CH}_3$  carbon is  $sp^3$ , the triple-bond carbons are  $sp$ , and the  $\text{C}\equiv\text{C}-\text{C}$  bond angle is approximately  $180^\circ$ .

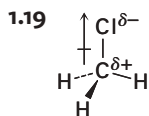
- 1.14 All carbons are  $sp^2$ , and all bond angles are approximately  $120^\circ$ .



- 1.16 (a) H (b) Br (c) Cl

- 1.17 (a) C is  $\delta^+$ , Br is  $\delta^-$  (b) C is  $\delta^+$ , N is  $\delta^-$   
 (c) H is  $\delta^+$ , N is  $\delta^-$  (d) C is  $\delta^+$ , S is  $\delta^-$   
 (e) Mg is  $\delta^+$ , C is  $\delta^-$  (f) C is  $\delta^+$ , F is  $\delta^-$

- 1.18  $\text{CCl}_4$  and  $\text{Cl}_2\text{O} < \text{TiCl}_3 < \text{MgCl}_2$



- 1.20 (a) Formic acid:  $K_a = 1.8 \times 10^{-4}$ ; picric acid:  $K_a = 0.42$   
 (b) Picric acid is stronger.

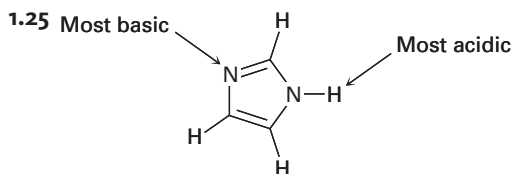
- 1.21 Water is the stronger acid.

- 1.22 (a) No (b) No

- 1.23 Lewis acids: (c), (d), (e); Lewis bases: (b), (f); both: (a)

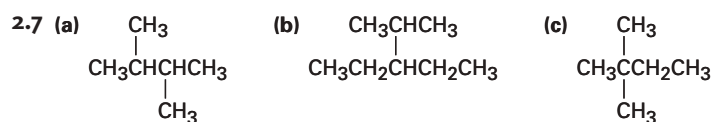
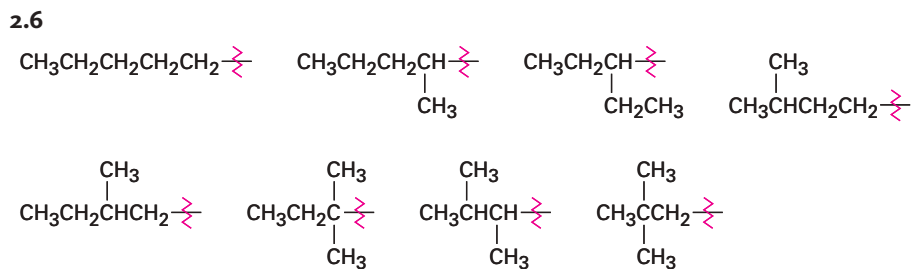
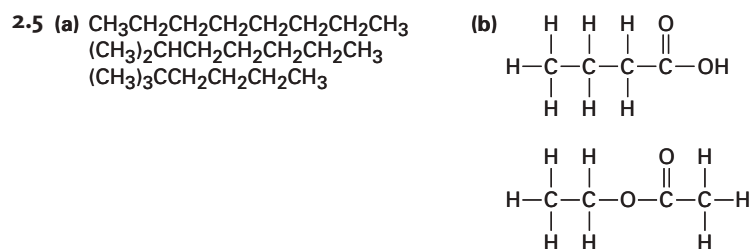
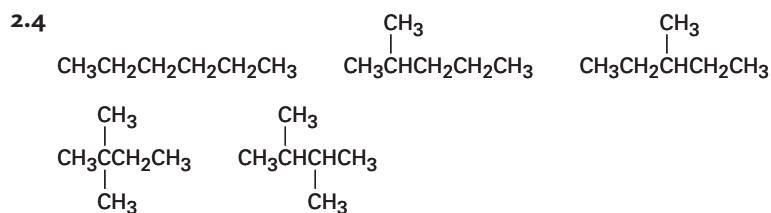
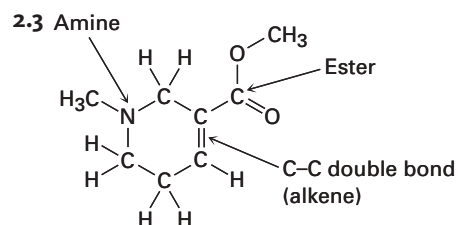
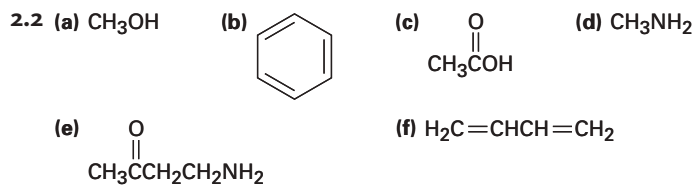
- 1.24 (a)  $\text{CH}_3\text{CH}_2\text{OH} + \text{HCl} \longrightarrow \text{CH}_3\text{CH}_2\text{OH}_2^+ \text{Cl}^-$ ;  
 $(\text{CH}_3)_2\text{NH} + \text{HCl} \longrightarrow (\text{CH}_3)_2\text{NH}_2^+ \text{Cl}^-$ ;  $(\text{CH}_3)_3\text{P} + \text{HCl} \longrightarrow$   
 $(\text{CH}_3)_3\text{PH}^+ \text{Cl}^-$

- (b)  $\text{HO}^- + \text{CH}_3^+ \longrightarrow \text{HO}-\text{CH}_3$ ;  $\text{HO}^- + \text{B}(\text{CH}_3)_3 \longrightarrow$   
 $\text{HO}-\text{B}(\text{CH}_3)_3^-$ ;  
 $\text{HO}^- + \text{MgBr}_2 \longrightarrow \text{HO}-\text{MgBr}_2^-$

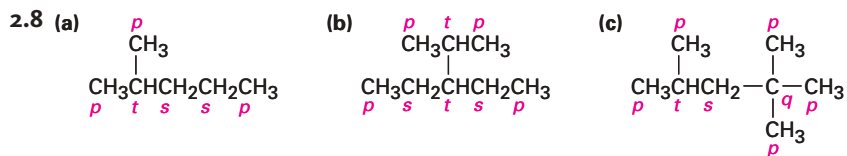


## Chapter 2

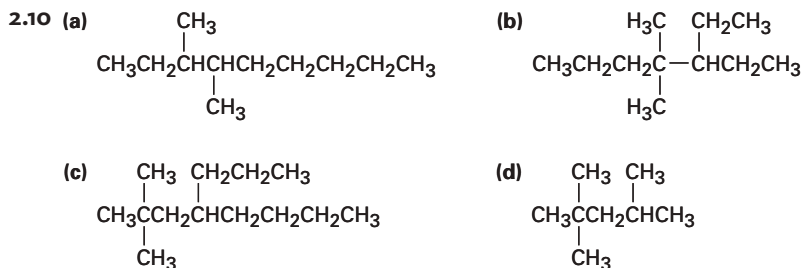
- 2.1 (a) Carboxylic acid, double bond  
 (b) Carboxylic acid, aromatic ring, ester  
 (c) Aldehyde, alcohol



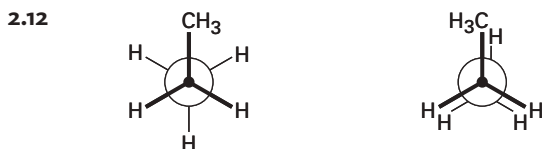




- 2.9 (a) Pentane, 2-methylbutane, 2,2-dimethylpropane  
 (b) 3,4-Dimethylhexane  
 (c) 2,4-Dimethylpentane  
 (d) 2,2,5-Trimethylheptane

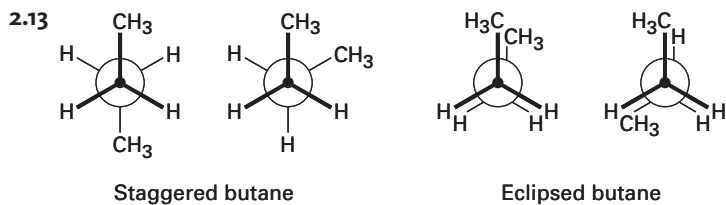


2.11 3,3,4,5-Tetramethylheptane



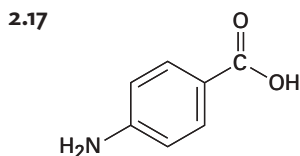
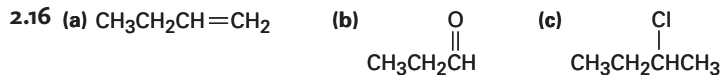
Most stable conformation  
(staggered)

Least stable conformation  
(eclipsed)

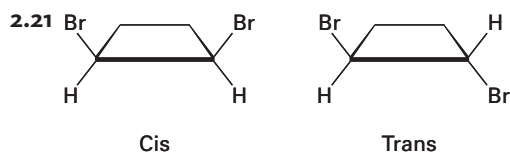
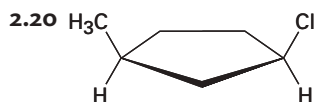
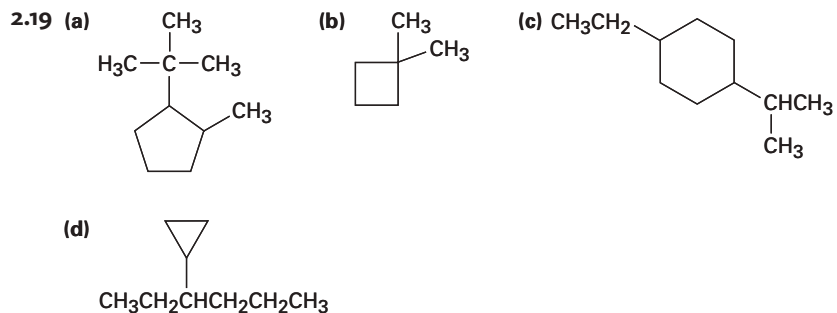


2.14 The first staggered conformation of butane is the most stable.

2.15 (a)  $\text{C}_5\text{H}_5\text{N}$       (b)  $\text{C}_6\text{H}_{10}\text{O}$       (c)  $\text{C}_8\text{H}_7\text{N}$

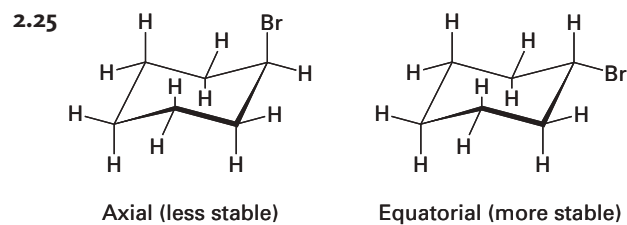
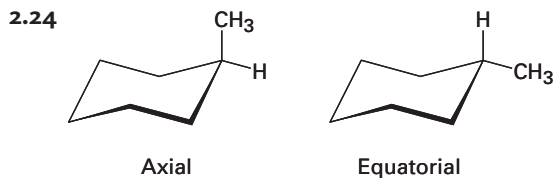


2.18 (a) 1,4-Dimethylcyclohexane      (b) 1-Ethyl-3-methylcyclopentane  
 (c) Isopropylcyclobutane

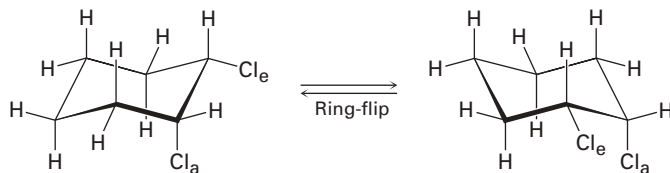


2.22 The two hydroxyl groups are cis; the two carbon chains are trans.

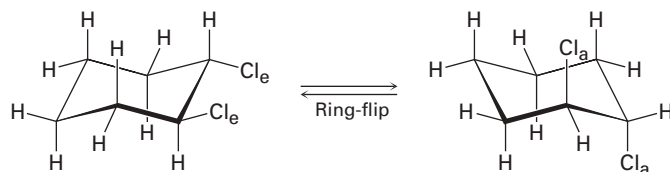
2.23 (a) *cis*-1,2-Dimethylcyclopentane  
 (b) *cis*-1-Bromo-3-methylcyclobutane



2.26 Axial and equatorial positions alternate on each side of a ring.



2.27 Axial and equatorial positions alternate on each side of a ring.

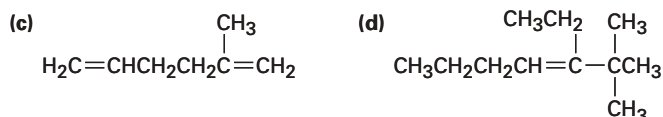
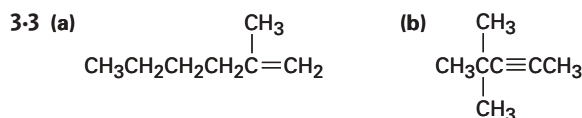


2.28 Less stable

### Chapter 3

3.1 (a) 3,4,4-Trimethylpent-1-ene (b) 3-Methylhex-3-yne  
(c) 4,7-Dimethylocta-2,5-diene (d) 6-Ethyl-7-methylnon-4-ene

3.2 (a) 1,2-Dimethylcyclohexene (b) 4,4-Dimethylcycloheptene  
(c) 3-Isopropylcyclopentene



3.4 (a) 2,5-Dimethylhex-3-yne (b) 3,3-Dimethylbut-1-yne  
(c) 3,3-Dimethyloct-4-yne (d) 2,5,5-Trimethylhept-3-yne

3.5 (a) 2,5,5-Trimethylhex-2-ene (b) 2,2-Dimethylhex-3-yne  
(c) 2-Methylhepta-2,5-diene (d) 1-Methylcyclopenta-1,3-diene

3.6 Compounds (c), (d), (e), and (f) can exist as pairs of isomers.

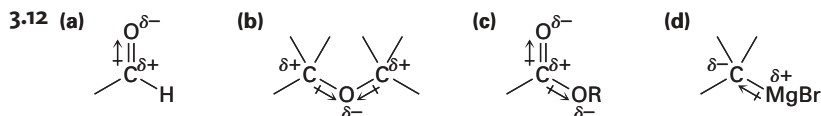
3.7 (a) *cis*-3,4-Dimethylhex-2-ene (b) *trans*-6-Methylhept-3-ene

3.8 (a) -Br (b) -Br (c) -CH<sub>2</sub>CH<sub>3</sub>  
(d) -OH (e) -CH<sub>2</sub>OH (f) -CH=O

3.9 (a) *Z* (b) *E* (c) *E*

3.10 *Z*

3.11 (a) Substitution (b) Elimination (c) Addition



3.13 Electrophile: (a), (c); nucleophile: (b), (d), (e)

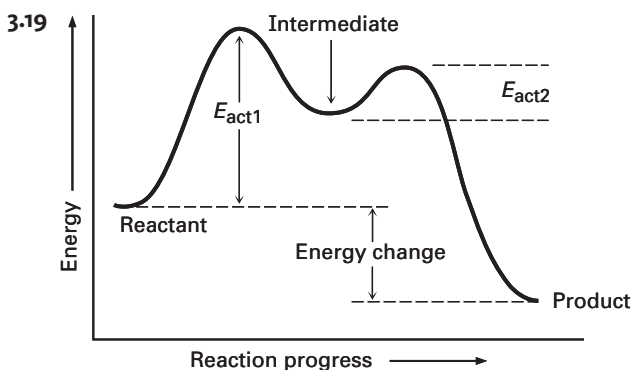
3.14 Boron is a Lewis acid/electrophile because it has only six outer-shell electrons.



3.15  $(\text{CH}_3)_3\text{C}^+$  is the intermediate.

3.16 2-Chloropentane and 3-chloropentane

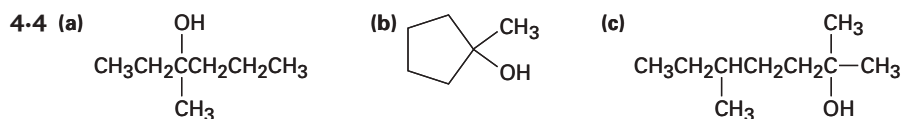
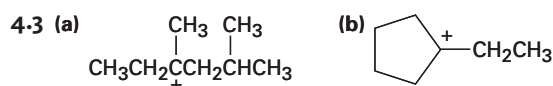
3.17  $E_{\text{act}} = 60 \text{ kJ/mol}$  is faster.



## Chapter 4

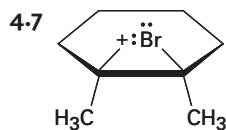
4.1 (a) Chlorocyclohexane (b) 2-Bromo-2-methylpentane  
(c) 4-Methylpentan-2-ol (d) 1-Bromo-1-methylcyclohexane

4.2 (a) Cyclopentene (b) 1-Ethylcyclohexene or ethylenecyclohexane  
(c) Hex-3-ene (d) Vinylcyclohexane (cyclohexylethylene)

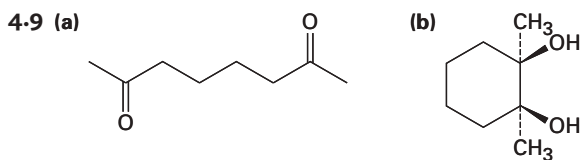


4.5 (a) But-1-ene or but-2-ene  
(b) 3-Methylpent-2-ene or 2-ethylbut-1-ene  
(c) 1,2-Dimethylcyclohexene or 2,3-dimethylcyclohexene

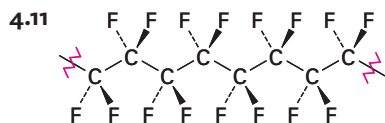
4.6 *trans*-1,2-Dibromo-1,2-dimethylcyclohexane



4.8 (a) 2-Methylpentane (b) 1,1-Dimethylcyclopentane

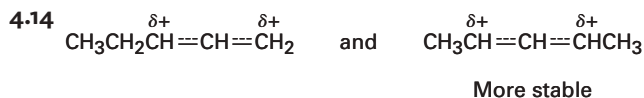


4.10 (a) 2-Methylpropene (b) Hex-3-ene

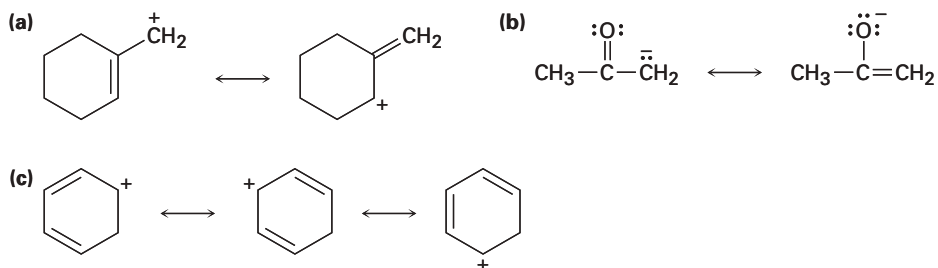


4.12 1,4-Dibromobut-2-ene and 3,4-dibromobut-1-ene

4.13 4-Chloropent-2-ene, 3-chloropent-1-ene, 1-chloropent-2-ene



4.15



4.16 (a) 6-Methylhept-3-yne (b) 3,3-Dimethylbut-1-yne  
 (c) 5-Methylhex-2-yne (d) Hept-2-en-5-yne

4.17 (a) 1,2-Dichloropent-1-ene  
 (b) 4-Bromohept-3-ene and 3-bromohept-3-ene  
 (c) *cis*-6-Methylhept-3-ene

4.18 Octan-4-one

4.19 (a) Pent-1-yne (b) Hex-3-yne

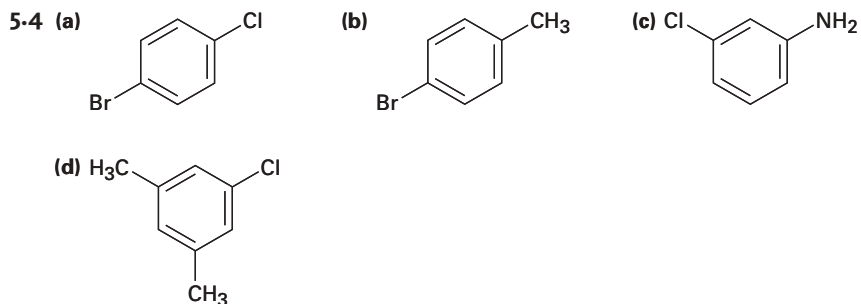
4.20 (a) 1-Bromo-3-methylbutane + acetylene  
 (b) 1-Bromopropane + prop-1-yne, or bromomethane + pent-1-yne  
 (c) Bromomethane + 3-methylbut-1-yne

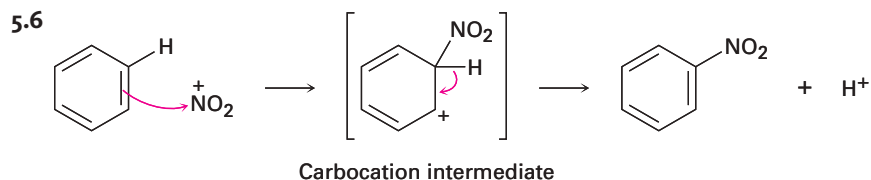
## Chapter 5

5.1 The two structures are resonance forms, not isomers.

5.2 (a) meta (b) para (c) ortho

5.3 (a) *m*-Bromochlorobenzene (b) (3-Methylbutyl)benzene  
 (c) *p*-Bromoaniline (d) 2,5-Dichlorotoluene  
 (e) 1-Ethyl-2,4-dinitrobenzene (f) 1,2,3,5-Tetramethylbenzene



5.5 *o*-, *m*-, and *p*-bromotoluene5.7 *p*-Xylene has one kind of ring position; *o*-xylene has two.

5.8 Three

5.9 (a) Ethylbenzene                      (b) 2-Ethyl-1,4-dimethylbenzene

5.10 (a) *tert*-Butylbenzene            (b) Propanoylbenzene, C<sub>6</sub>H<sub>5</sub>COCH<sub>2</sub>CH<sub>3</sub>

5.11 (a) Nitrobenzene &lt; toluene &lt; phenol

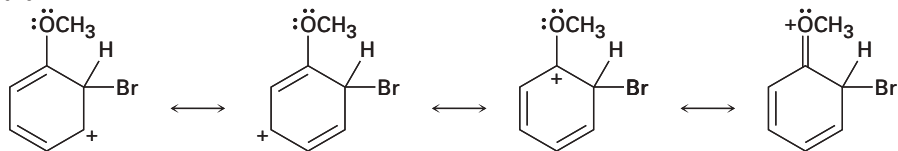
(b) Benzoic acid &lt; chlorobenzene &lt; benzene &lt; phenol

(c) Benzaldehyde &lt; bromobenzene &lt; benzene &lt; aniline

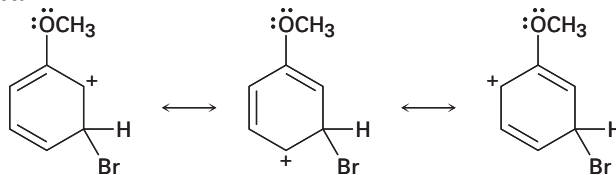
5.12 (a) *m*-Chlorobenzonitrile        (b) *o*- and *p*-Bromochlorobenzene5.13 (a) *m*-Nitrobenzenesulfonic acid(b) *o*- and *p*-Bromobenzenesulfonic acid(c) *o*- and *p*-Methylbenzenesulfonic acid(d) *m*-Carboxybenzenesulfonic acid(e) *m*-Cyanobenzenesulfonic acid

5.14

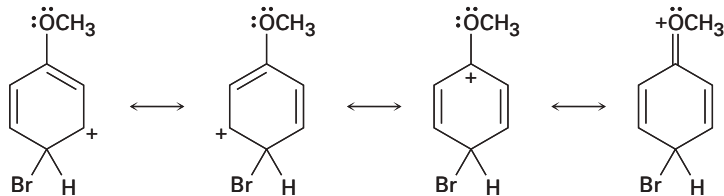
Ortho



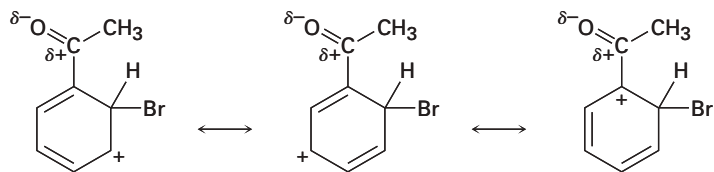
Meta



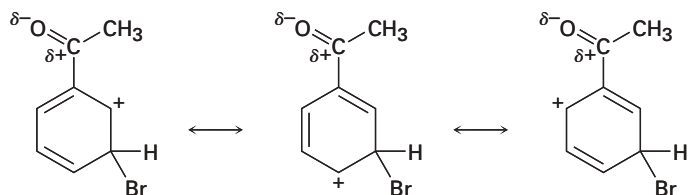
Para



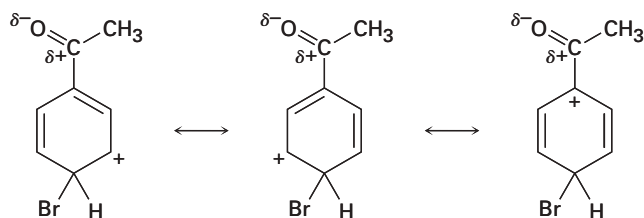
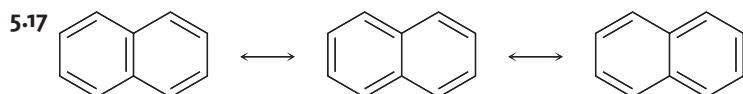
## 5.15 Ortho



## Meta



## Para

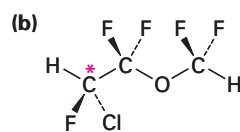
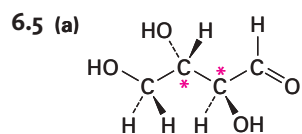
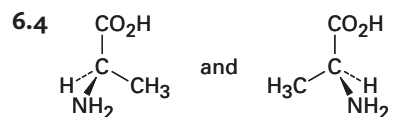
5.16 (a) *m*-Chlorobenzoic acid      (b) *o*-Benzenedicarboxylic acid5.18 (a) 1.  $\text{CH}_3\text{Cl}$ ,  $\text{AlCl}_3$ ; 2.  $\text{CH}_3\text{COCl}$ ,  $\text{AlCl}_3$ (b) 1.  $\text{Cl}_2$ ,  $\text{FeCl}_3$ ; 2.  $\text{HNO}_3$ ,  $\text{H}_2\text{SO}_4$ 5.19 (a) 1.  $\text{Br}_2$ ,  $\text{FeBr}_3$ ; 2.  $\text{CH}_3\text{Cl}$ ,  $\text{AlCl}_3$       (b) 1. 2  $\text{CH}_3\text{Cl}$ ,  $\text{AlCl}_3$ ; 2.  $\text{Br}_2$ ,  $\text{FeBr}_3$ 5.20 1.  $\text{CH}_3\text{Cl}$ ,  $\text{AlCl}_3$ ; 2.  $\text{KMnO}_4$ ,  $\text{H}_2\text{O}$ ; 3.  $\text{Cl}_2$ ,  $\text{FeCl}_3$ 

## Chapter 6

6.1 Chiral: screw, shoe

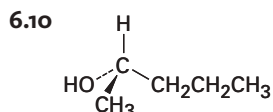
6.2 Chiral: (b), (c)

6.3 Chiral: (b)



6.6 Levorotatory

6.7 +16.1

6.8 (a) -OH, -CH<sub>2</sub>CH<sub>2</sub>OH, -CH<sub>2</sub>CH<sub>3</sub>, -H(b) -OH, -CO<sub>2</sub>CH<sub>3</sub>, -CO<sub>2</sub>H, -CH<sub>2</sub>OH(c) -NH<sub>2</sub>, -CN, -CH<sub>2</sub>NHCH<sub>3</sub>, -CH<sub>2</sub>NH<sub>2</sub>(d) -SSCH<sub>3</sub>, -SH, -CH<sub>2</sub>SCH<sub>3</sub>, -CH<sub>3</sub>6.9 (a) *S* (b) *S* (c) *R*6.11 *S*6.12 (a) *R,R* (b) *S,R* (c) *R,S*

6.13 Molecules (b) and (c) are enantiomers (mirror images). Molecule (a) is the diastereomer of (b) and (c).

6.14 (a) *R,R* (b) *S,R* (c) *R,S* (d) *S,S*

6.15 6 Stereocenters; 64 stereoisomers

6.16 *S,S*

6.17 Meso: (a) and (c)

6.18 Meso: (a) and (c)

6.19 The product is the pure *S* ester.

6.20 (a) Constitutional isomers (b) Diastereomers

## Chapter 7

7.1 (a) 2-Bromobutane (b) 3-Chloro-2-methylpentane  
 (c) 1-Chloro-3-methylbutane (d) 1,3-Dichloro-3-methylbutane  
 (e) 1-Bromo-4-chlorobutane (f) 4-Bromo-1-chloropentane

7.2 (a) CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>C(CH<sub>3</sub>)<sub>2</sub>CH(Cl)CH<sub>3</sub>  
 (b) CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>C(Cl)<sub>2</sub>CH(CH<sub>3</sub>)<sub>2</sub>  
 (c) CH<sub>3</sub>CH<sub>2</sub>C(Br)(CH<sub>2</sub>CH<sub>3</sub>)<sub>2</sub>  
 (d) CH<sub>3</sub>CH(Cl)CH<sub>2</sub>CH(CH<sub>3</sub>)CH(Br)CH<sub>3</sub>

7.3 1-Chloro-3-methylpentane, 2-chloro-3-methylpentane, 3-chloro-3-methylpentane, 3-(chloromethyl)pentane. The first two are chiral.

7.4 (a) 2-Methylpropan-2-ol + HCl (b) 4-Methylpentan-2-ol + PBr<sub>3</sub>  
 (c) 5-Methylhexan-1-ol + PBr<sub>3</sub> (d) 2,4-Dimethylhexan-2-ol + HCl

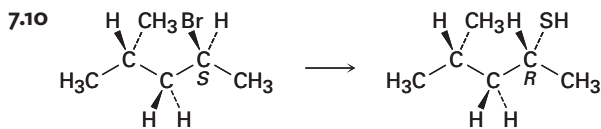
7.5 (a) 4-Bromo-2-methylhexane (b) 1-Chloro-3,3-dimethylcyclopentane

7.6 (a) CH<sub>3</sub>CH<sub>2</sub>CH(I)CH<sub>3</sub> (b) (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>SH (c) C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>CN7.7 (a) 1-Bromobutane + NaOH (b) 1-Bromo-3-methylbutane + NaN<sub>3</sub>

7.8 (a) Rate is tripled. (b) Rate is quadrupled.

7.9 (*R*) CH<sub>3</sub>CO<sub>2</sub>CH(CH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>





- 7.11 (a) Reaction with  $\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$  is faster.  
 (b) Reaction with  $(\text{CH}_3)_2\text{CHCH}_2\text{Cl}$  is faster.

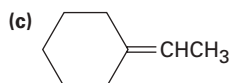
7.12  $\text{CH}_3\text{I} > \text{CH}_3\text{Br} > \text{CH}_3\text{F}$

7.13 (a) Rate is unchanged. (b) Rate is doubled.

7.14 Racemic 3-bromo-3-methyloctane

7.15 The *S* substrate gives a racemic mixture of alcohols.

7.16 (a) 2-Methylpent-2-ene (b) 2,3,5-Trimethylhex-2-ene



7.17 (a) 1-Bromo-3,6-dimethylheptane

(b) 1,2-Dimethyl-4-bromocyclopentane

7.18 The rate is tripled.

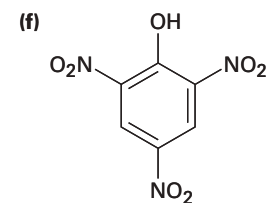
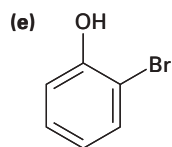
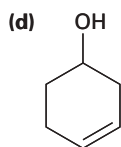
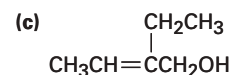
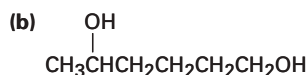
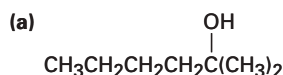
7.19 (a)  $\text{S}_{\text{N}}2$  (b) E2 (c)  $\text{S}_{\text{N}}1$  (d) E1cB

## Chapter 8

- 8.1 (a) 5-Methylhexane-2,4-diol (b) 2-Methyl-4-phenylbutan-2-ol  
 (c) 4,4-Dimethylcyclohexanol (d) *trans*-2-Bromocyclopentanol  
 (e) 4-Bromo-3-methylphenol (f) 3-Methoxycyclopentene

8.2 Secondary: (a), (c), (d); tertiary: (b)

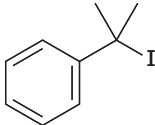
8.3



- 8.4 (a) Diisopropyl ether  
 (b) Cyclopentyl propyl ether  
 (c) *p*-Bromoanisole or 4-bromo-1-methoxybenzene  
 (d) Ethyl isobutyl ether

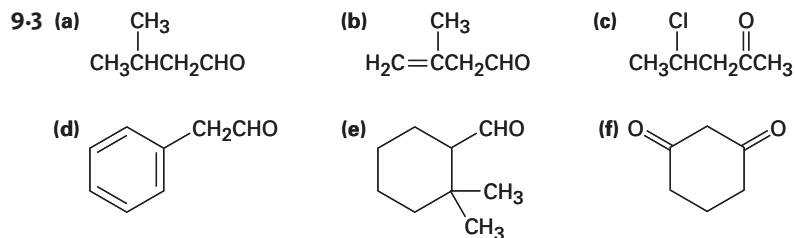
8.5 (a)  $\text{NaBH}_4$  (b)  $\text{LiAlH}_4$

- 8.6 (a)  $\text{C}_6\text{H}_5\text{CHO}$ ,  $\text{C}_6\text{H}_5\text{CO}_2\text{H}$ ,  $\text{C}_6\text{H}_5\text{CO}_2\text{R}$   
 (b)  $\text{C}_6\text{H}_5\text{COCH}_3$   
 (c) Cyclohexanone

- 8.7 (a) 1-Methylcyclopentanol  
 (b) 1,1-Diphenylethanol  
 (c) 3-Methylhexan-3-ol
- 8.8 (a) Acetone +  $\text{CH}_3\text{MgBr}$   
 (b) Cyclohexanone +  $\text{CH}_3\text{MgBr}$   
 (c) Pentan-3-one +  $\text{CH}_3\text{MgBr}$ , or butan-2-one +  $\text{CH}_3\text{CH}_2\text{MgBr}$
- 8.9 (a) 2,3-Dimethylpent-2-ene (b) 2-Methylpent-2-ene
- 8.10 (a) 2,3-Dimethylcyclohexanol (b) Heptan-4-ol
- 8.11 (a) 1-Phenylethanol (b) 2-Methylpropan-1-ol (c) Cyclopentanol
- 8.12 (a) Cyclohexanone (b) Hexanoic acid (c) Hexan-2-one
- 8.13 (a) Cyclohexanone (b) Hexanal (c) Hexan-2-one
- 8.14 (a)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{O}^- + \text{CH}_3\text{Br}$   
 (b)  $\text{C}_6\text{H}_5\text{O}^- + \text{CH}_3\text{Br}$   
 (c)  $(\text{CH}_3)_2\text{CHO}^- + \text{C}_6\text{H}_5\text{CH}_2\text{Br}$
- 8.15 (a) Bromoethane > chloroethane > 2-bromopropane > 2-chloro-2-methylpropane
- 8.16  $\text{CH}_3\text{CH}_2\text{COCH}_2\text{CH}(\text{CH}_3)_2$ ;  
 (i)  $\text{CH}_3\text{CH}_2\text{CH}(\text{OCH}_3)\text{CH}_2\text{CH}(\text{CH}_3)_2$   
 (ii)  $\text{CH}_3\text{CH}_2\text{CH}(\text{Cl})\text{CH}_2\text{CH}(\text{CH}_3)_2$   
 (iii)  $\text{CH}_3\text{CH}_2\text{COCH}_2\text{CH}(\text{CH}_3)_2$
- 8.17 (a)  +  $\text{CH}_3\text{OH}$  (b)  $\begin{array}{c} \text{CH}_3 \\ | \\ \text{CH}_3\text{CH}_2\text{CHOH} \end{array} + \text{CH}_3\text{CH}_2\text{CH}_2\text{I}$
- 8.18 The product is a racemic mixture of *R,R* and *S,S* butane-1,2-diols.
- 8.19 (a) Butane-2-thiol (b) 2,2,6-Trimethylheptane-4-thiol  
 (c) Cyclopent-2-ene-1-thiol (d) Ethyl isopropyl sulfide  
 (e) *o*-Di(methylthio)benzene (f) 3-(Ethylthio)cyclohexanone
- 8.20 (a) 1.  $\text{PBr}_3$ ; 2.  $\text{Na}^+ \text{ } ^-\text{SH}$  (b) 1.  $\text{LiAlH}_4$ ; 2.  $\text{PBr}_3$ ; 3.  $\text{Na}^+ \text{ } ^-\text{SH}$

## Chapter 9

- 9.1 (a) Pentan-2-one (b)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCHO}$   
 (c)  $\text{CH}_3\text{CH}_2\text{COCH}_2\text{CH}_2\text{CHO}$  (d) Cyclopentanone
- 9.2 (a) 2-Methylpentan-3-one  
 (b) 3-Phenylpropanal  
 (c) Octane-2,6-dione  
 (d) *trans*-2-Methylcyclohexanecarbaldehyde  
 (e) Pentanedial  
 (f) *cis*-2,5-Dimethylcyclohexanone



9.4 (a) Periodinane

(b) 1. LiAlH<sub>4</sub>; 2. periodinane

(c) 1. KMnO<sub>4</sub>; 2. LiAlH<sub>4</sub>; 3. periodinane

9.5 (a) Periodinane (b) H<sub>3</sub>O<sup>+</sup>, HgSO<sub>4</sub> (c) KMnO<sub>4</sub>, H<sub>3</sub>O<sup>+</sup>

9.6 (a) 1. H<sub>3</sub>O<sup>+</sup>; 2. periodinane (b) 1. CH<sub>3</sub>COCl, AlCl<sub>3</sub>; 2. NaBH<sub>4</sub>

9.7 (a) Pentanoic acid

(b) 2,2-Dimethylhexanoic acid

(c) No reaction

9.8 (CH<sub>3</sub>)<sub>2</sub>C(OH)CN

9.9 (CH<sub>3</sub>)<sub>2</sub>C(OH)OCH<sub>3</sub>

9.10 (a) C<sub>5</sub>H<sub>9</sub>MgBr + (CH<sub>3</sub>)<sub>2</sub>CHCHO or (CH<sub>3</sub>)<sub>2</sub>CHMgBr + C<sub>5</sub>H<sub>9</sub>CHO  
or C<sub>5</sub>H<sub>9</sub>COCH(CH<sub>3</sub>)<sub>2</sub> + NaBH<sub>4</sub>

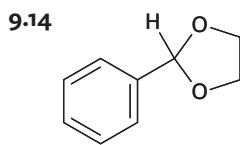
(b) PhCH<sub>2</sub>CHO + NaBH<sub>4</sub> or PhCH<sub>2</sub>CO<sub>2</sub>R + LiAlH<sub>4</sub> or PhCH<sub>2</sub>MgBr + CH<sub>2</sub>O

(c) C<sub>6</sub>H<sub>11</sub>MgBr + (CH<sub>3</sub>)<sub>2</sub>C=O or CH<sub>3</sub>MgBr + C<sub>6</sub>H<sub>11</sub>CO<sub>2</sub>R  
or CH<sub>3</sub>MgBr + C<sub>6</sub>H<sub>11</sub>COCH<sub>3</sub>

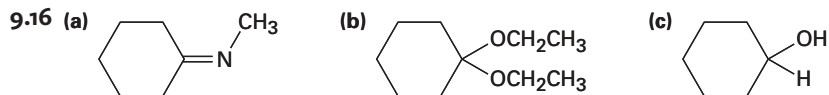
9.11 C<sub>5</sub>H<sub>9</sub>COCH<sub>3</sub> + CH<sub>3</sub>MgBr or C<sub>5</sub>H<sub>9</sub>MgBr + (CH<sub>3</sub>)<sub>2</sub>C=O

9.12 Labeled water adds reversibly to the carbonyl group.

9.13 The mechanism of acetal formation is shown in Figure 9.3.



9.15 1. CH<sub>3</sub>OH, acid catalyst; 2. CH<sub>3</sub>MgBr; 3. H<sub>3</sub>O<sup>+</sup>



9.17 (CH<sub>3</sub>)<sub>2</sub>CHCOCH<sub>2</sub>CH<sub>3</sub> + CH<sub>3</sub>NH<sub>2</sub>

9.18 6-Methylcyclohex-2-enone + (CH<sub>3</sub>)<sub>2</sub>CHOH

## Chapter 10

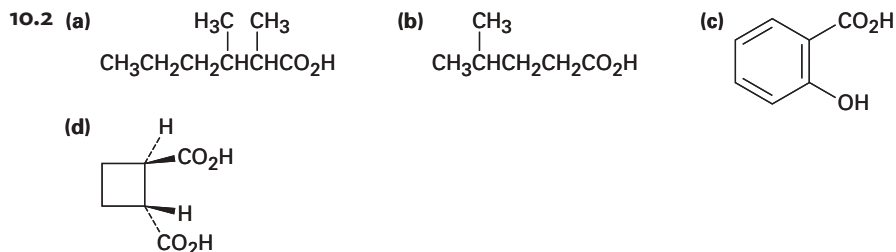
10.1 (a) 3-Methylbutanoic acid

(b) 4-Bromopentanoic acid

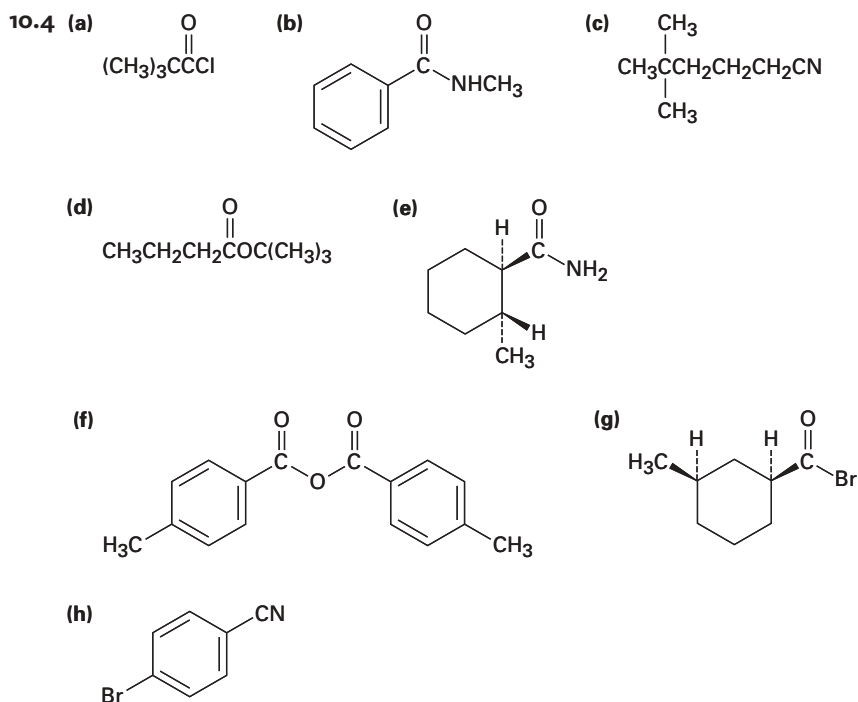
(c) 2-Ethylpentanoic acid

(d) *cis*-Hex-4-enoic acid

(e) *cis*-Cyclopentane-1,3-dicarboxylic acid



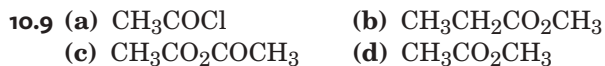
- 10.3 (a) 4-Methylpentanoyl chloride  
 (b) Cyclohexylacetamide  
 (c) Isopropyl 2-methylpropanoate  
 (d) Benzoic anhydride  
 (e) Isopropyl cyclopentanecarboxylate  
 (f) Cyclopentyl 2-methylpropanoate  
 (g) *N*-Methylpent-4-enamide  
 (h) 2-Methylbutanenitrile

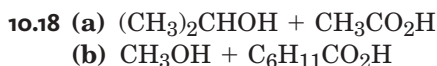
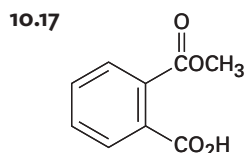
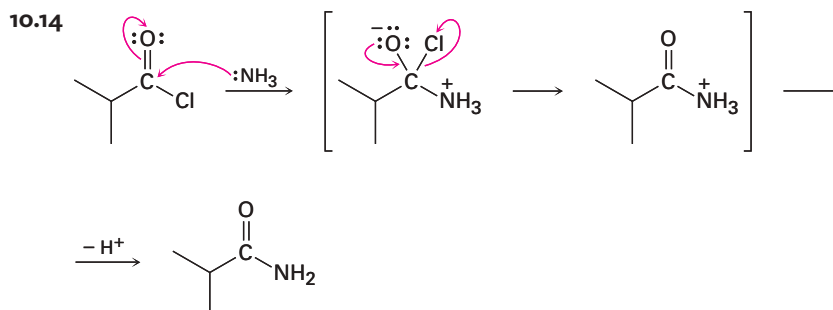
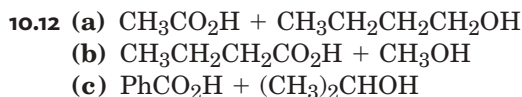
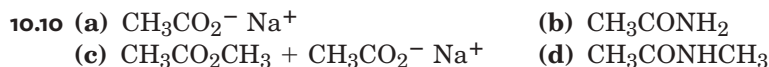


- 10.6 (a) Methanol < phenol < *p*-nitrophenol < acetic acid < sulfuric acid  
 (b) Ethanol < benzoic acid < *p*-cyanobenzoic acid

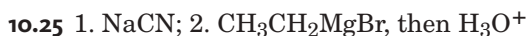
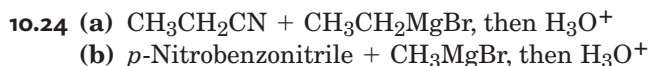
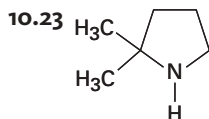
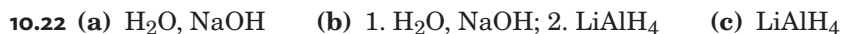
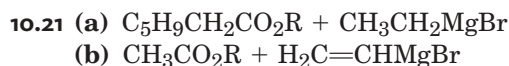
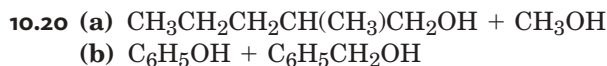
10.7 Lactic acid is stronger because of the electron-withdrawing effect of the -OH group.

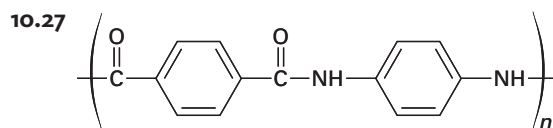
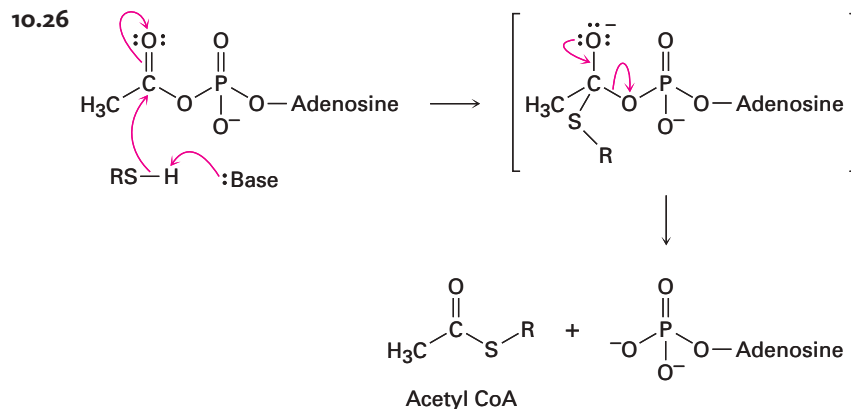
10.8 1. NaCN; 2. NaOH, H<sub>2</sub>O. Iodobenzene cannot be converted to benzoic acid by this method.





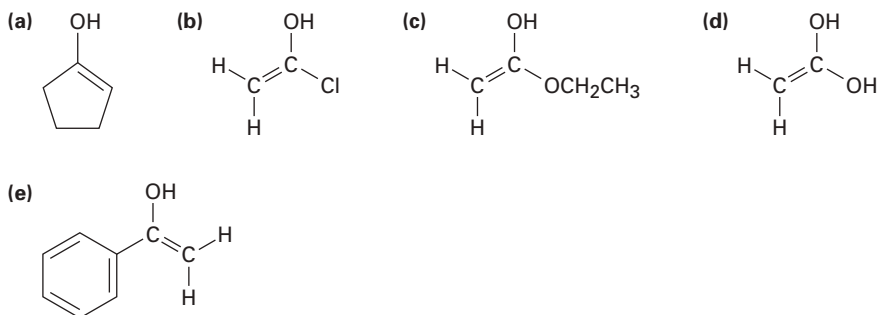
10.19 Reaction of an acid with an alkoxide ion gives the unreactive carboxylate ion.



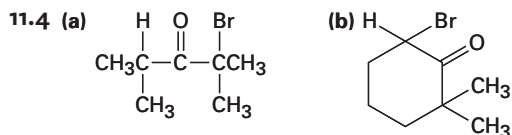
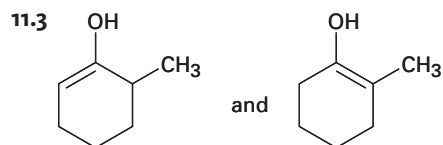


## Chapter 11

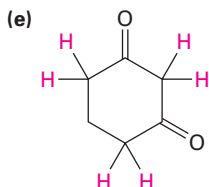
11.1

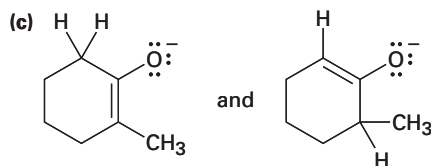
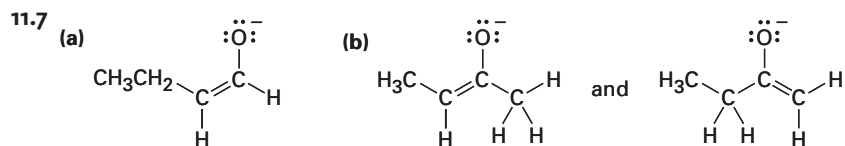


11.2 (a) 4 (b) 3 (c) 3 (d) 4 (e) 3

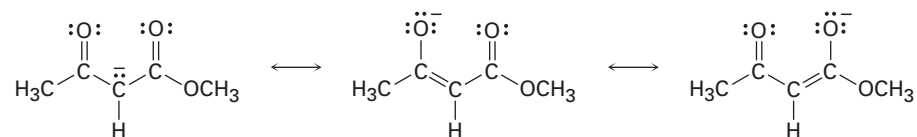
11.5 1.  $\text{Br}_2$ ; 2. Pyridine, heat

11.6 (a)  $\text{CH}_3\text{CH}_2\text{CHO}$  (b)  $(\text{CH}_3)_3\text{CCOCH}_3$   
 (c)  $\text{CH}_3\text{CO}_2\text{H}$  (d)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}\equiv\text{N}$





11.8



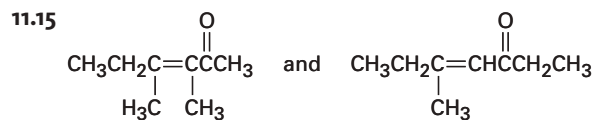
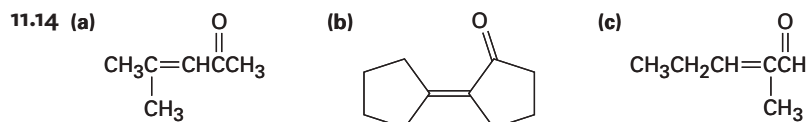
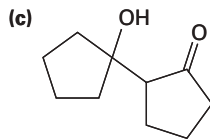
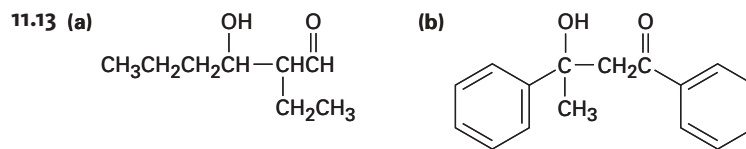
11.9 (a)  $\text{CH}_3\text{CH}_2\text{Br}$  (b)  $\text{C}_6\text{H}_5\text{CH}_2\text{Br}$  (c)  $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{Br}$

11.10 (a) 1.  $\text{Na}^+ \text{ } ^-\text{OEt}$ ; 2.  $(\text{CH}_3)_2\text{CHCH}_2\text{Br}$ ; 3.  $\text{H}_3\text{O}^+$

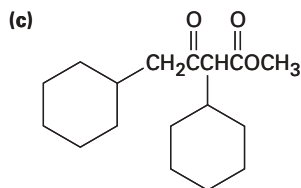
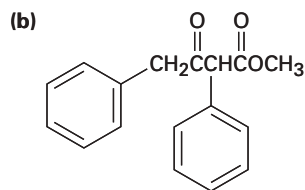
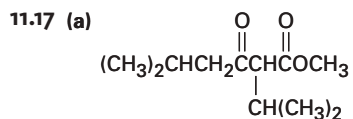
(b) 1.  $\text{Na}^+ \text{ } ^-\text{OEt}$ ; 2.  $\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$ ; 3.  $\text{Na}^+ \text{ } ^-\text{OEt}$ ; 4.  $\text{CH}_3\text{Br}$ ; 5.  $\text{H}_3\text{O}^+$

11.11 1.  $\text{Na}^+ \text{ } ^-\text{OEt}$ ; 2.  $(\text{CH}_3)_2\text{CHCH}_2\text{Br}$ ; 3.  $\text{Na}^+ \text{ } ^-\text{OEt}$ ; 4.  $\text{CH}_3\text{Br}$ ; 5.  $\text{H}_3\text{O}^+$

11.12 Only (a) can undergo an aldol reaction.

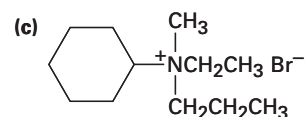
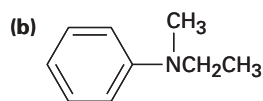
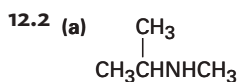


11.16 Only (c) undergoes a Claisen reaction.



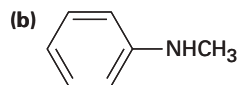
## Chapter 12

12.1 (a) Primary (b) Secondary (c) Tertiary

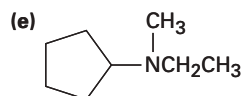
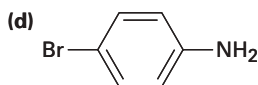


12.3 (a) Isopropylamine (b) Diethylamine  
(c) *N*-Methylpyrrole (d) *N*-Methyl-*N*-ethylcyclohexylamine  
(e) Diisopropylamine (f) Butane-1,3-diamine

12.4 (a)  $(\text{CH}_3\text{CH}_2)_3\text{N}$



(c)  $(\text{CH}_3\text{CH}_2)_4\text{N}^+ \text{Br}^-$



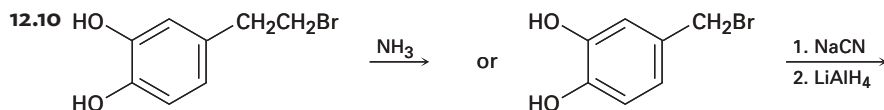
12.5 *N*-Methylcyclopentylammonium bromide

12.6 (a)  $\text{CH}_3\text{CH}_2\text{NH}_2$  (b) NaOH (c)  $\text{CH}_3\text{NHCH}_3$  (d)  $(\text{CH}_3)_3\text{N}$

12.7 (a)  $\text{CH}_3\text{CH}_2\text{CONH}_2$  (b)  $\text{CH}_3\text{CH}_2\text{CONHCH}_2\text{CH}_2\text{CH}_3$   
(c)  $\text{PhCONH}_2$

12.8 (a)  $(\text{CH}_3)_2\text{CHCH}_2\text{CN}$  (b) PhCN

12.9 (a)  $3 \text{CH}_3\text{CH}_2\text{Br} + \text{NH}_3$  (b)  $4 \text{CH}_3\text{Br} + \text{NH}_3$



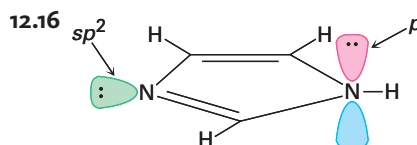
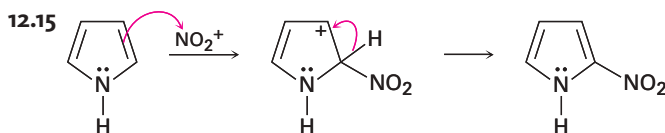
12.11 (a)  $\text{CH}_3\text{CH}_2\text{NH}_2 + \text{CH}_3\text{COCH}_3$  or  $(\text{CH}_3)_2\text{CHNH}_2 + \text{CH}_3\text{CHO}$   
(b)  $\text{C}_6\text{H}_5\text{NH}_2 + \text{CH}_3\text{CHO}$   
(c)  $\text{C}_5\text{H}_{11}\text{NH}_2 + \text{CH}_2\text{O}$  or  $\text{CH}_3\text{NH}_2 + \text{cyclopentanone}$

12.12  $(\text{CH}_3)_2\text{NH} + o\text{-methylbenzaldehyde}$

12.13 (a) 1.  $\text{CH}_3\text{Cl}$ ,  $\text{AlCl}_3$ ; 2.  $\text{KMnO}_4$ ,  $\text{H}_2\text{O}$ ; 3.  $\text{HNO}_3$ ,  $\text{H}_2\text{SO}_4$ ; 4.  $\text{H}_2$ , Pt catalyst  
(b) 1.  $\text{HNO}_3$ ,  $\text{H}_2\text{SO}_4$ ; 2.  $\text{H}_2/\text{Pt}$  catalyst; 3. 3 Br<sub>2</sub>



- 12.14 (a) *N*-Methyl-2-bromopyrrole (b) *N*-Methyl-2-methylpyrrole  
(c) *N*-Methyl-2-acetylpyrrole



12.17 The pyridine-like doubly bonded nitrogen is more basic.

12.18 The side-chain nitrogen is more basic than the ring nitrogen.

## Chapter 13

13.1 I<sub>2</sub>

13.2 Butanoic acid

13.3 IR:  $\epsilon = 2.0 \times 10^{-19}$  J; X ray:  $\epsilon = 6.6 \times 10^{-17}$  J

13.4  $\lambda = 9.0 \times 10^{-6}$  m is higher in energy.

13.5 (a) 0.16 m (b)  $7.5 \times 10^{-4}$  kJ/mol; much less energy than light

13.6 (a) Ketone or aldehyde (b) Nitro  
(c) Nitrile or alkyne (d) Carboxylic acid  
(e) Alcohol and ester

13.7 (a) CH<sub>3</sub>CH<sub>2</sub>OH has an -OH absorption.  
(b) Hex-1-ene has a double-bond absorption.  
(c) Propanoic acid has a very broad -OH absorption.

13.8 Nitrile: 2210–2260 cm<sup>-1</sup>; ketone: 1690 cm<sup>-1</sup>; double bond: 1640 cm<sup>-1</sup>

13.9  $3 \times 10^{-5}$  M

13.10 (a), (c), (d), and (f) have UV absorptions.

13.11 Hexa-1,3,5-triene absorbs at a longer wavelength.

13.12 The energy used by NMR spectroscopy is less than that used by IR spectroscopy.

13.13 (a) <sup>1</sup>H, 1; <sup>13</sup>C, 1 (b) <sup>1</sup>H, 1; <sup>13</sup>C, 1 (c) <sup>1</sup>H, 2; <sup>13</sup>C, 2  
(d) <sup>1</sup>H, 1; <sup>13</sup>C, 1 (e) <sup>1</sup>H, 1; <sup>13</sup>C, 1 (f) <sup>1</sup>H, 1; <sup>13</sup>C, 1  
(g) <sup>1</sup>H, 2; <sup>13</sup>C, 2 (h) <sup>1</sup>H, 2; <sup>13</sup>C, 2 (i) <sup>1</sup>H, 1; <sup>13</sup>C, 2

13.14 The vinylic C–H protons are nonequivalent.

13.15 <sup>1</sup>H, 5; <sup>13</sup>C, 7

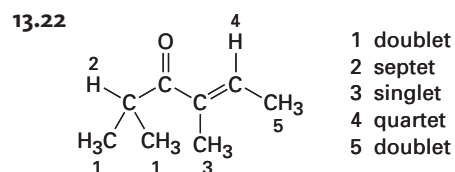
13.16 (a) 210 Hz (b) 2.1  $\delta$  (c) 460 Hz

13.17 (a) 7.27  $\delta$  (b) 3.05  $\delta$  (c) 3.47  $\delta$  (d) 5.30  $\delta$

13.18 (a) 0.88  $\delta$  (b) 2.17  $\delta$  (c) 7.17  $\delta$  (d) 2.22  $\delta$

13.19 Two peaks; 3:2 ratio

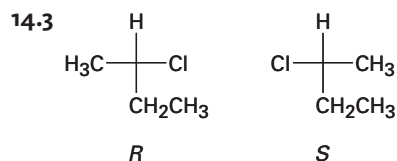
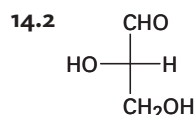
- 13.20 (a)  $-\text{CHBr}_2$ , quartet;  $-\text{CH}_3$ , doublet  
 (b)  $\text{CH}_3\text{O}^-$ , singlet;  $-\text{OCH}_2^-$ , triplet;  $-\text{CH}_2\text{Br}$ , triplet  
 (c)  $\text{ClCH}_2^-$ , triplet;  $-\text{CH}_2^-$ , quintet  
 (d)  $\text{CH}_3^-$ , triplet;  $-\text{CH}_2^-$ , quartet;  $-\text{CH}^-$ , septet;  $(\text{CH}_3)_2$ , doublet  
 (e)  $\text{CH}_3^-$ , triplet;  $-\text{CH}_2^-$ , quartet;  $-\text{CH}^-$ , septet;  $(\text{CH}_3)_2$ , doublet  
 (f)  $=\text{CH}$ , triplet;  $-\text{CH}_2^-$ , doublet; aromatic C-H, two multiplets
- 13.21 (a)  $\text{CH}_3\text{OCH}_3$  (b)  $\text{CH}_3\text{CO}_2\text{CH}_3$  (c)  $(\text{CH}_3)_2\text{CHCl}$



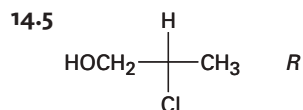
- 13.23 (a) 1 (b) 5 (c) 4 (d) 7 (e) 5 (f) 7
- 13.24 (a) Hept-1-ene  
 (b) 2-Methylpentane  
 (c) 1-Chloro-2-methylpropane

## Chapter 14

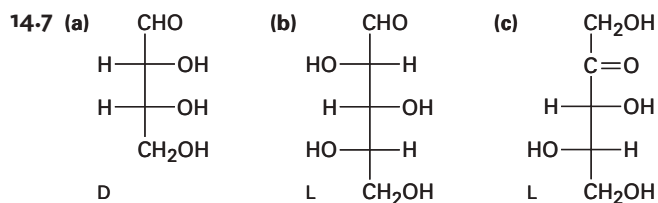
- 14.1 (a) Aldotetrose (b) Ketopentose  
 (c) Ketohehexose (d) Aldopentose

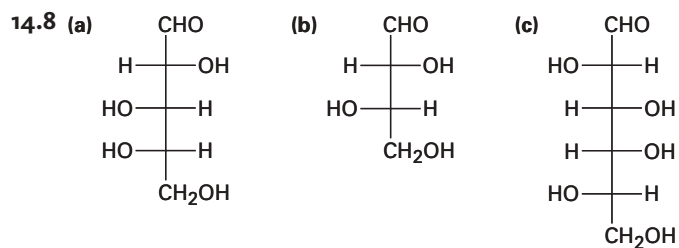


- 14.4 (a) *S* (b) *R* (c) *S*

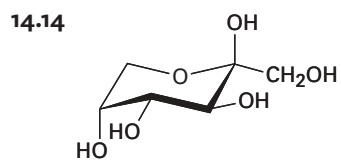
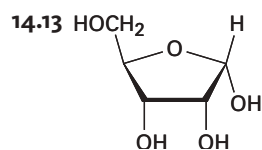
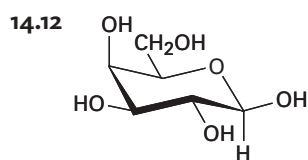
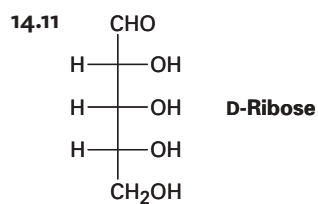
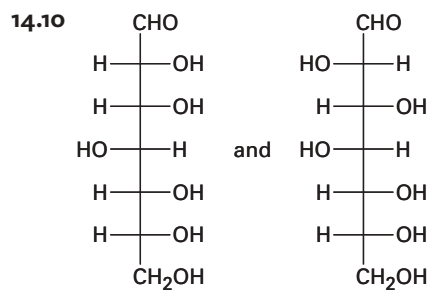


- 14.6 (a) L (b) D (c) D

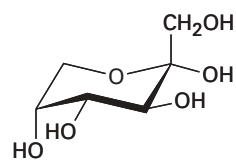




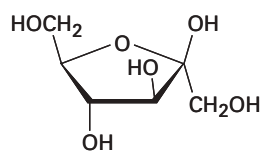
14.9 There are 16 D and 16 L aldoheptoses.



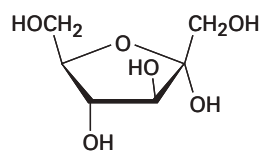
$\beta$ -D-Fructopyranose



$\alpha$ -D-Fructopyranose

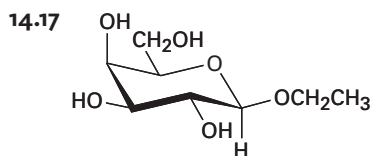
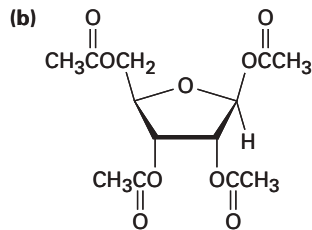
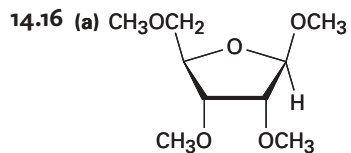
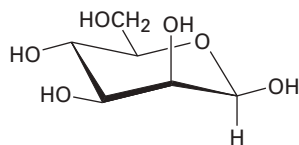


$\beta$ -D-Fructofuranose



$\alpha$ -D-Fructofuranose

## 14.15 Equal stability

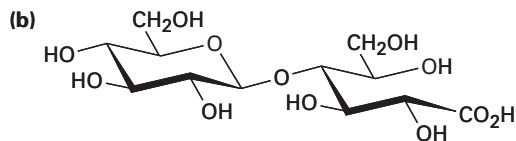
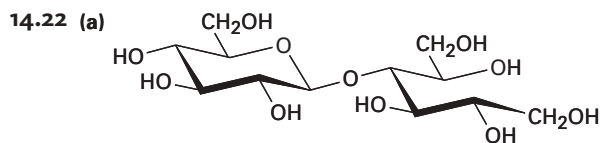


14.18 D-Galactitol is a meso compound.

14.19 An alditol has a  $-\text{CH}_2\text{OH}$  group at both ends; either could have been a  $-\text{CHO}$  group in the parent sugar.

14.20 D-Allaric acid is a meso compound; D-glucaric acid is not.

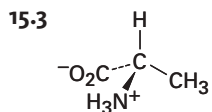
14.21 D-Allose and D-galactose yield meso aldaric acids; the other six D-aldohexoses yield optically active aldaric acids.



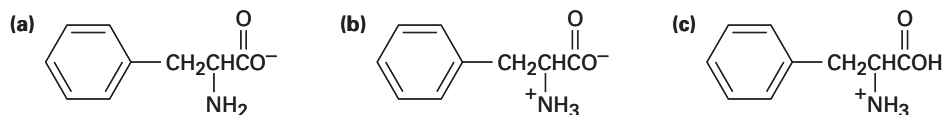
## Chapter 15

15.1 Aromatic: Phe, Tyr, Trp, His; sulfur-containing: Cys, Met; alcohols: Ser, Trp; hydrocarbon side chains: Ala, Ile, Leu, Val.

15.2 The sulfur atom in the  $-\text{CH}_2\text{SH}$  group of cysteine makes the side chain higher ranked than the  $-\text{CO}_2\text{H}$  group.



15.4



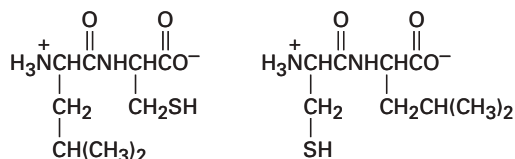
15.5 (a) Toward (+): Glu &gt; Val; toward (-): none

(b) Toward (+): Phe; toward (-): Gly

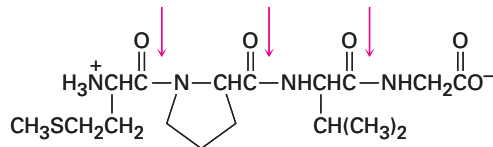
(c) Toward (+): Phe &gt; Ser; toward (-): none

15.6 Net positive at pH = 5.3; net negative at pH = 7.3

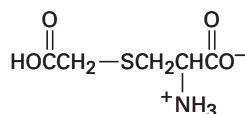
15.7


 15.8 Val-Tyr-Gly (VYG), Tyr-Gly-Val (YGV), Gly-Val-Tyr (GVY),  
Val-Gly-Tyr (VGY), Tyr-Val-Gly (YVG), Gly-Tyr-Val (GYV)

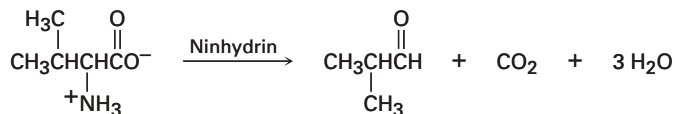
15.9



15.10



15.11



15.12 Trypsin: Asp-Arg + Val-Tyr-Ile-His-Pro-Phe

Chymotrypsin: Asp-Arg-Val-Tyr + Ile-His-Pro-Phe

15.13 Arg-Pro-Leu-Gly-Ile-Val

15.14 Methionine

15.15 (1) Protect the amino group of leucine.

(2) Protect the carboxylic acid group of alanine.

(3) Couple the protected amino acids with DCC.

(4) Remove the leucine protecting group.

(5) Remove the alanine protecting group.

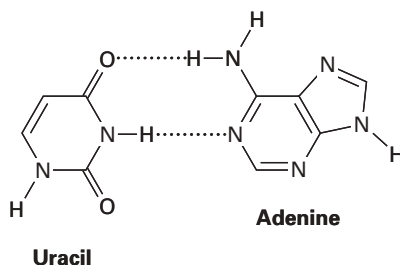
 15.16 This is a typical nucleophilic acyl substitution reaction, with the amine of the amino acid as the nucleophile and *tert*-butyl carbonate as the leaving group. The *tert*-butyl carbonate then loses CO<sub>2</sub> and gives *tert*-butoxide, which is protonated.

15.17 (a) Lyase (b) Hydrolase (c) Oxidoreductase

## Chapter 16

- 16.1  $\text{CH}_3(\text{CH}_2)_{18}\text{CO}_2\text{CH}_2(\text{CH}_2)_{30}\text{CH}_3$
- 16.2 Glycerol monooleate distearate is higher melting.
- 16.3 The fat molecule with stearic acid esterified to the central  $-\text{OH}$  group of glycerol has no chiral centers and is optically inactive.
- 16.4  $[\text{CH}_3(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_7\text{CO}_2^-]_2 \text{Mg}^{2+}$
- 16.5 Glycerol dioleate monopalmitate  $\rightarrow$  glycerol + 2 sodium oleate + sodium palmitate
- 16.6 Two ketones, double bond
- 16.7 Both have an aromatic ring.
- 16.10 (3') CCGATTAGGCA (5') or (5') ACGGATTAGCC (3')

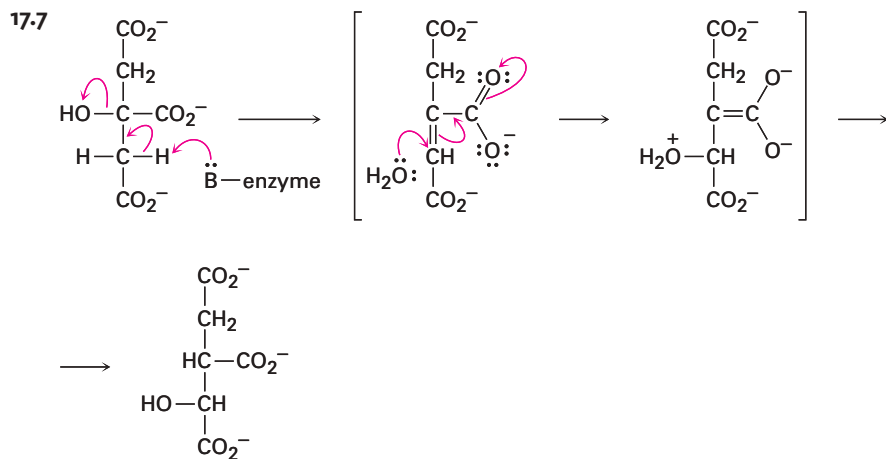
16.11



- 16.12 (3') CUA AUGGCAU (5') or (5') UACGGUAAUC (3')
- 16.13 (3') AAGCGTCTCA (5') or (5') ACTCTGCGAA (3')
- 16.14 (a) GCU, GCC, GCA, GCG (b) UUU, UUC  
(c) UUA, UUG, CUU, CUC, CUA, CUG (d) UAU, UAC
- 16.15 Leu-Met-Ala-Trp-Pro-Stop
- 16.16 (3') GAA-UAC-CGA-ACC-GGG-AUU (5')
- 16.17 (3') GAA-TAC-CGA-ACC-GGG-ATT (5')

## Chapter 17

- 17.1  $\text{HOCH}_2\text{CH}(\text{OH})\text{CH}_2\text{OH} + \text{ATP} \rightarrow \text{HOCH}_2\text{CH}(\text{OH})\text{CH}_2\text{OPO}_3^{2-} + \text{ADP}$
- 17.3 (a) 8 acetyl CoA; 7 passages (b) 10 acetyl CoA; 9 passages
- 17.4 Steps 7 and 10
- 17.5 Step 1: nucleophilic acyl substitution at phosphorus;  
step 2: isomerization by keto-enol tautomerization;  
step 3: like step 1;  
step 4: retro aldol condensation;  
step 5: like step 2;  
step 6: oxidation;  
step 7: like step 2;  
step 8: isomerization;  
step 9: E1cB reaction;  
step 10: substitution at phosphorus, followed by tautomerization
- 17.6 Citrate and isocitrate



17.9 Asparagine

Boldfaced references refer to pages where terms are defined.

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