1. Web sites
2. Chemical Composition & Bonding
3. Chemical Terms
4. Functional Groups
5. Configuration
   - Z & E
   - Stereochemistry
   - Presentation of Structure (Perspective Diagram, Ball-and Stick, Space-filling)
   - Rules
6. Conformation
7. Configuration & Conformation determine interaction between biomolecules
8. Chemical Reactivity
   - Hydrocarbons
   - Activation of hydrocarbons
   - Five general reactions between biomolecules

   Oxidation-reduction

   Cleavage and formation of C-C bonds

   Internal rearrangement

   Group Transfer

   Condensation reaction
9. Evolution of Biomolecules

Web Links

http://www.biology.arizona.edu/biochemistry/biochemistry.html
http://www.umass.edu/microbio/rasmol/rastut.htm
http://www.cryst.bbk.ac.uk/PPS2/
http://www.genomicglossaries.com/content/biomolecules.asp
http://www.indstate.edu/thcme/mwking/biomolecules.html
http://www.chem.qmul.ac.uk/iupac/
http://www.acdlabs.com/iupac/nomenclature/
http://www.biochemweb.org/general.shtml
http://www.worthpublishers.com/lehninger3d/

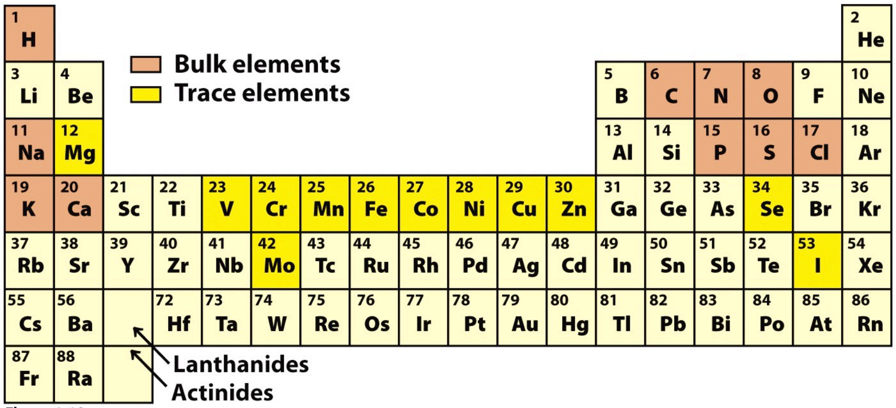

Figure 1-12
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Elements Found in the Earth's Crust, Ocean and Atmosphere

Earth's Crust	*(by mass)*	Oceans	*(by mass)*	Atmosphere	*(volume of dry air)*
Oxygen	46.5%	Oxygen	85.79%	Nitrogen	78.08%
Silicon	28.0%	Hydrogen	10.67%	Oxygen	20.95%
Aluminum	8.1%	Chlorine	2.07%	Argon	0.93%
Iron	5.1%	Sodium	1.14%	Carbon Dioxide	0.03%
Calcium	3.5%	Magnesium	0.14%	Neon	0.0018%
Sodium	3.0%	All Others	0.19%	Helium	0.0005%
Potassium	2.5%			Krypton	0.0001%
Magnesium	2.2%			Hydrogen	0.00005%
Titanium	0.5%			Xenon	0.000008%

Elements of the Human Body

Element	% of Body	Functional Significance
Oxygen	65.0	A major contributor to both organic and inorganic molecules; as a gas it is necessary for the production of cellular energy.
Carbon	18.5	**The main component of all organic molecules, i.e. carbohydrates, lipids, proteins, and nucleic acids.**
Hydrogen	10.0	Another component of all organic molecules; in its ionic form it is influential on the pH of body fluids.
Nitrogen	3.0	An important structural component of all genetic material (nucleic acids).
Calcium	1.2	A building block of bones and teeth; its ionic form is essential in muscle contraction, impulse conduction in nerves, and blood clotting.
Phosphorus	1.0	Joins calcium to contribute to bone crystalline structure; present in nucleic acids and ATP.
Potassium	0.4	Its ionic form is the major cation (positive ions) in cells; necessary for conduction of nerve impulses and muscle contraction.
Sulfur	0.3	**Important component of muscle proteins**
Sodium	0.2	
Chlorine	0.2	In ionic form is the most abundant anion (negative ion) outside the cell.
Magnesium	0.1	Found in bone and plays an important assisting role in many metabolic functions.
Iodine	0.1	Required in thyroid hormones which are the body's main metabolic hormones.
Iron	0.1	Basic building block of the hemoglobin molecule which is a major transporter of oxygen in body.

A number of factors have been associated with the occurrence of a deficiency of a mineral in humans: deficiency in the soil; water and plants; mineral imbalances; processing of water or soil; and, inadequate dietary intake.

Acid-Dependent Minerals That Require Adequate Stomach Acid to Enhance Intraluminal Absorption in the Small Intestine

Chromium	Copper	Iron	Magnesium
Manganese	Molybdenum	Selenium	Zinc

The lack of minerals in our soil is evidenced through the need for constant fertilization. Plants need nitrogen, hydrogen, oxygen, chlorine, carbon, boron, sulfur, potassium, magnesium, phosphorus, iron, zinc, copper manganese, and molybdenum, some of which are commonly replaced through fertilizers to provide maximum crops through minimum investment. However, humans are known to additionally need calcium, sodium, fluorine, bromine, chromium, iodine, silicon, selenium, beryllium, lithium, cobalt, vanadium and nickel, which would not necessarily be replaced through fertilization for plants.

Trace Elements of the Human Body

Element	Functional Significance
Chromium	Promotes glucose metabolism; helps regulate blood sugar. (Deficiency: atherosclerosis, heart disease, skin)
Cobalt	Promotes normal red-blood cell formation.
Copper	Promotes normal red-blood cell formation; acts as a catalyst in storage and formation; acts as a catalyst in storage and release of iron to form hemoglobin; promotes connective tissue formation and central nervous system function.
Fluorine	Prevents dental caries
Manganese	Promotes normal growth and development; promotes cell function; helps many body enzymes generate energy.
Molybedenum	Promotes normal growth and development and cell function.
Selenium	Complements Vitamin E to act as an efficient anti-oxidant.
Vanadium	Plays role in metabolism of bones and teeth.
Zinc	Maintains normal taste and smell; aids wound healing; helps synthesize DNA and RNA.

Functions of Manganese

1. activates numerous enzymes,
2. helps in the utilization of thiamin,
3. helps in the utilization of vitamin E (tocopherol),
4. helps in the utilization of iron, and
5. increases the level of the antioxidant, superoxide dismutase (SOD)

Deficiency will cause the following problems

1. heart disease
2. dermatitis
3. lower levels of the good cholesterol fraction, HDL-cholesterol
4. accelerated bone loss
5. reduced fertility
6. retarded growth in children
7. low blood sugar
8. middle ear problems, including difficulty maintaining balance

Boron Function

brain function, especially in enhancing memory, cognitive function, and hand-eye coordination.

Insufficient: Arthritis

Selenium

Functions:

1. protect against harmful exposure to the heavy metal, mercury
2. help make a vital antioxidant, glutathione
3. help regulate male hormones
4. in males, support prostate function
5. work synergistically with vitamin E
6. enhance immune function

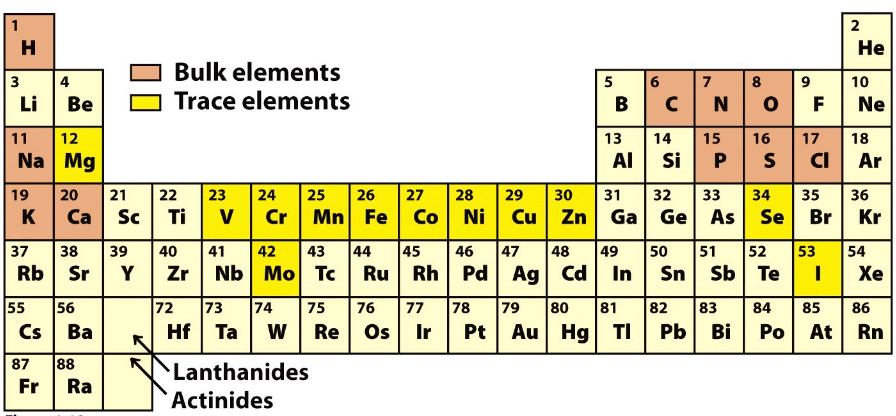
Deficiency can contribute to many conditions, including:

1. dry skin
2. dandruff
3. the development of cataracts
4. fatigue

affect the efficiency of vitamin E utilization

Recommended Dietary Allowances of Minerals for Healthy Adults

Age (Years)	Ca (g)	P (mg)	Mg (mg)	Fe (mg)	Zn (mg)	Cu (μg)	I (μg)	Se (μg)	Mo (μg)	Mn (mg)	F (mg)	Cr (μg)
Males												
19-30	1.0	700	400	8	11	900	150	55	45	2.3	4	36
31-50	1.0	700	420	8	11	900	150	55	45	2.3	4	36
51-70	1.2	700	420	8	11	900	150	55	45	2.3	4	30
> 70	1.2	700	420	8	11	900	150	55	45	2.3	4	30
Females												
19-30	1.0	700	310	18	8	900	150	55	45	1.8	3	25
31-50	1.0	700	320	18	8	900	150	55	45	1.8	3	25
51-70	1.0	700	320	8	8	900	150	55	45	1.8	3	25
> 70	1.0	700	320	8	8	900	150	55	45	1.8	3	25
Pregnant	~1.3	1250	400	27	12	1000	220	60	50	2.0	4	30
Nursing	~1.3	1250	350	10	13	1300	290	70	50	2.6	4	45



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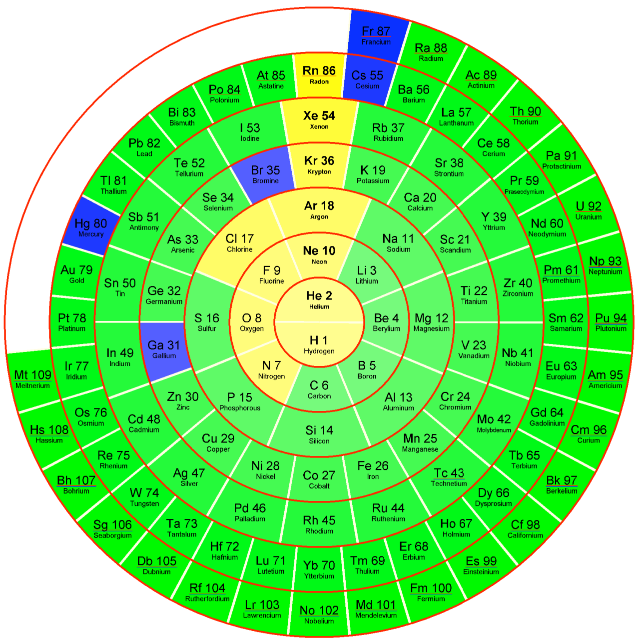
Mayan Periodic Chart of the Elements



The Mayan Periodic Table of Elements, named for its similarity to an ancient calendar, is based on electron shells. The shells are shown as concentric circles. This arrangement shows some aspects of the elements better than the traditional table.

1. The reactivity of elements. The noble gases are shown in bold type in the vertical row above the center of the chart. This is the ideal state for an atom. Each of the elements wants to be there. The elements closest to the noble gases are so close they can taste it. This makes them more eager, more reactive, since all they need is to gain or lose one electron. As you move away from the noble gases along the concentric circles, the elements get less and less reactive, since they are so far from being a noble gas, they don't really think it is worth the effort.

2. The proportions of compounds. The proportion of elements can be guessed by looking at the 'hops' that an element must take to get to the noble gases. The guideline is that for elements to combine, one should be from the left and one from the right. The number of hops an atom takes to get to the vertical line must equal the number its partner on the other side takes. If they are not equal, increase the number of atoms until they are equal.

For example, Sodium just has one hop to the left to get to the vertical line. One the opposite side Chlorine also just has one hop to get there. This implies they may combine in a one-to-one ratio. Aluminum needs three hops left to get vertical, and Oxygen needs just two. Since the number of hops needs to be the same on both sides, we need two Aluminum atoms and three Oxygen to make it equal. This implies Al(2)O(3) is a good possibility for a compound.

3. Transition elements. The transition elements are are usually shown as a block of elements apart from the others. The Mayan arrangement shows them to be real elements, not just an afterthought.

Legend:
Radioactive elements are underlined in red.
Synthetic elements are underlined in blue.
The physical state at standard temperature and pressure:

Liquid
Solid
Gas

by Mitch Fincher, mitchfincher@yahoo.com 2000/09/18

table 3-2

The Electronegativities of Some Elements

Element	Electronegativity*
F	4.0
O	3.5
Cl	3.0
N	3.0
Br	2.8
S	2.5
C	2.5
I	2.5
Se	2.4
P	2.1
H	2.1
Cu	1.9
Fe	1.8
Co	1.8
Ni	1.8
Mo	1.8
Zn	1.6
Mn	1.5
Mg	1.2
Ca	1.0
Li	1.0
Na	0.9
K	0.8

*The higher the number, the more electronegative (the greater the electron affinity of) the element.

THE THREE PRIMARY OR STRONG BONDS

- Metal to Non-Metal: Ionic
- Non-Metal to Non-Metal: Covalent
- Metal to Metal: Metallic

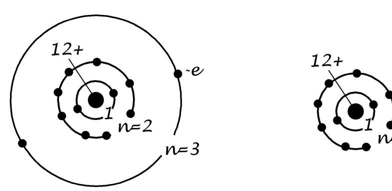
THE IONIC BOND

- The establishment of the "Noble gas configuration" by electron transfer from metallic atoms to non-metallic atoms. The electrostatic bond is thus formed between positively charged metallic ions (cations), and negatively charged ions (anions).
- Ionic bonds are <u>non-directional.</u>

THE IONIC BOND

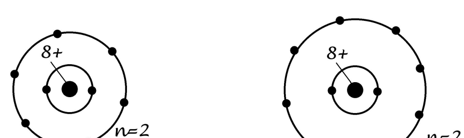
- **Always produces <u>compounds</u>. Examples include NaCl (common salt), Na_2O (natron) and magnesium oxide (MgO), where one species is metallic (the cation) and is from groups I-III or the transition metals: the other species is non-metallic (the anion),[*] and is from Groups V, VI or VII. Most importantly, ionically bonded solids are non-metallic and inorganic – they are ceramics.**
  - *** A Negative ION.**

RUTHERFORD-BOHR MODELS



a) Magnesium Atom
Atomic Radius, r = 0.16 nm

b) Magnesium Cation (Mg^{2+})
r = 0.06 nm



c) Oxygen Atom
r = 0.078nm

d) Oxygen Cation (O^{2-})
r = 0.132nm

THE METALLIC BOND

- **The bonds formed between an array of positively charged metallic cations and a "sea" of negatively charged, free-electrons, the latter being "donated" from the outer shells of the constituent atoms.**
- **Metallic bonds are <u>non-directional.</u>**
- **Occurs for all metallic elements and their alloys (i.e., Group I, I and III metals and for the transition metals), to form close-packed solids**

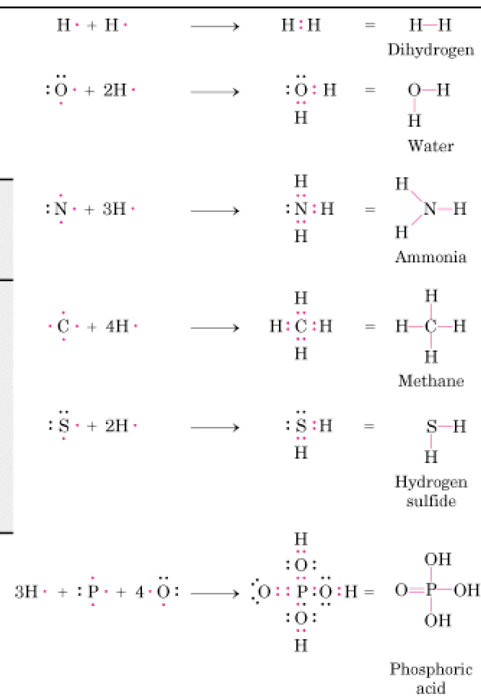
THE COVALENT BOND

- **The attainment of the "magical octet" of outer shell electrons by atoms sharing pairs of valence electrons.**
- **Each shared electron pair constitutes a single bond.**
- **Covalent bonds are <u>directional.</u>**

THE COVALENT BOND

- Occurs in non-metallic (Groups IV, V, VI and VII) elements to form e.g., network solids (diamond carbon and silicon) and molecular gases (hydrogen, oxygen).
- Covalent bonding also occurs in compounds, as in the network solids SiC (both Group IV elements), and SiO_2 (Groups IV and VI respectively) and molecular gases (e.g., carbon dioxide).

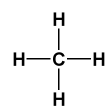
Atom	Number of unpaired electrons (in red)	Number of electrons in complete outer shell
H·	1	2
:Ö·	2	8
:N·	3	8
·C·	4	8
:S·	2	8
:P·	3	8

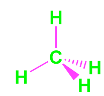


Electronic configuration of Carbon C $1s^2 2s^2 2p^2$

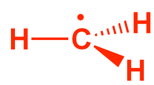
- *Covalent bonds*: sharing of electrons between atoms
- Carbon: can accept 4 electrons from other atoms, i.e., Carbon is tetravalent (valency = 4)

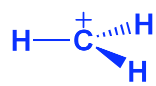
Methane: CH_4

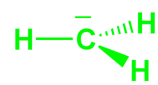




Chemistry: Inert







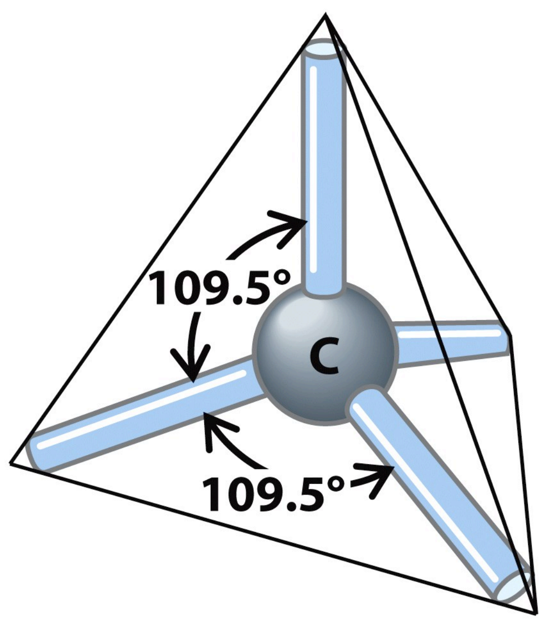


Figure 1-14a
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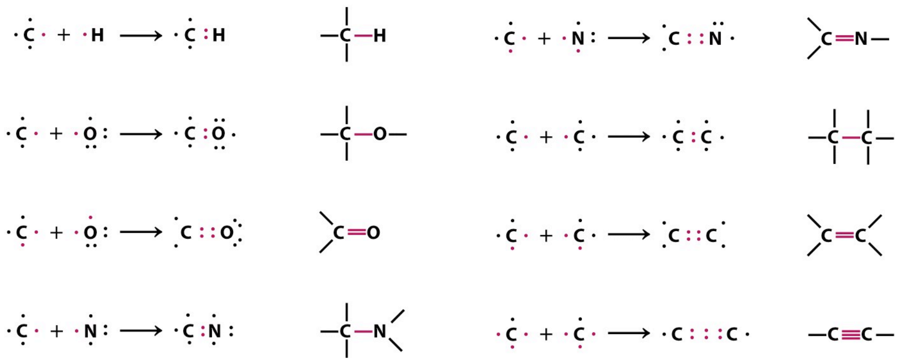

Figure 1-13
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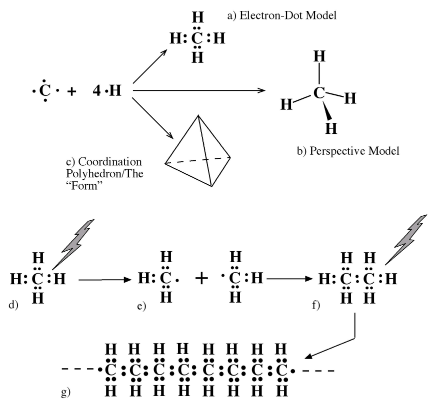
table 3–3

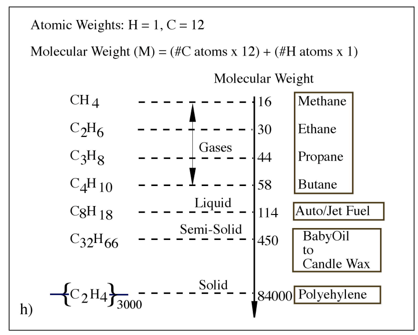
Strengths of Bonds Common in Biomolecules

Type of bond	Bond dissociation energy* (kJ/mol)	Type of bond	Bond dissociation energy (kJ/mol)
Single bonds		Double bonds	
O—H	461	C═O	712
H—H	435	C═N	615
P—O	419	C═C	611
C—H	414	P═O	502
N—H	389		
C—O	352	Triple bonds	
C—C	348	C≡C	816
S—H	339	N≡N	930
C—N	293		
C—S	260		
N—O	222		
S—S	214		

*The greater the energy required for bond dissociation (breakage), the stronger the bond.

THE METHANE MOLECULE, PARAFFINS AND MOLECULAR WEIGHT





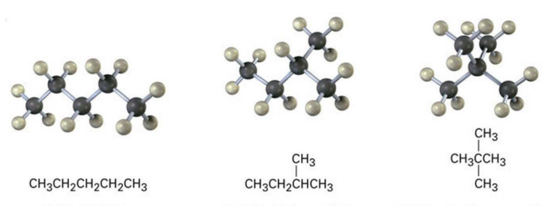
Alkanes and Alkane Isomers

Isomers

- From the Greek *isos* + *meros* meaning "made of the same parts"
- Compounds that have the same molecular formula but different structures

Table 3.2
Number of Alkane Isomers

Formula	Number of isomers
C_6H_{14}	5
C_7H_{16}	9
C_8H_{18}	18
C_9H_{20}	35
$C_{10}H_{22}$	75
$C_{15}H_{32}$	4,347
$C_{20}H_{42}$	366,319
$C_{30}H_{62}$	4,111,846,763



$CH_3CH_2CH_2CH_2CH_3$ **Pentane, C_5H_{12}**

$CH_3CH_2CH(CH_3)CH_3$ **2-Methylbutane, C_5H_{12}**

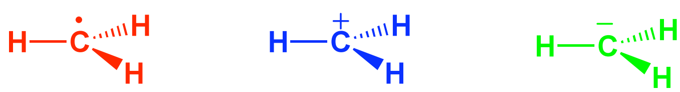
$CH_3C(CH_3)_2CH_3$ **2,2-Dimethylpropane, C_5H_{12}**

Electronic configuration of Carbon   C $1s^2 2s^2 2p^2$

- *Covalent bonds*: sharing of electrons between atoms
- Carbon: can accept 4 electrons from other atoms, i.e.,
  Carbon is tetravalent (valency = 4)

Methane: CH_4

Chemistry: Inert



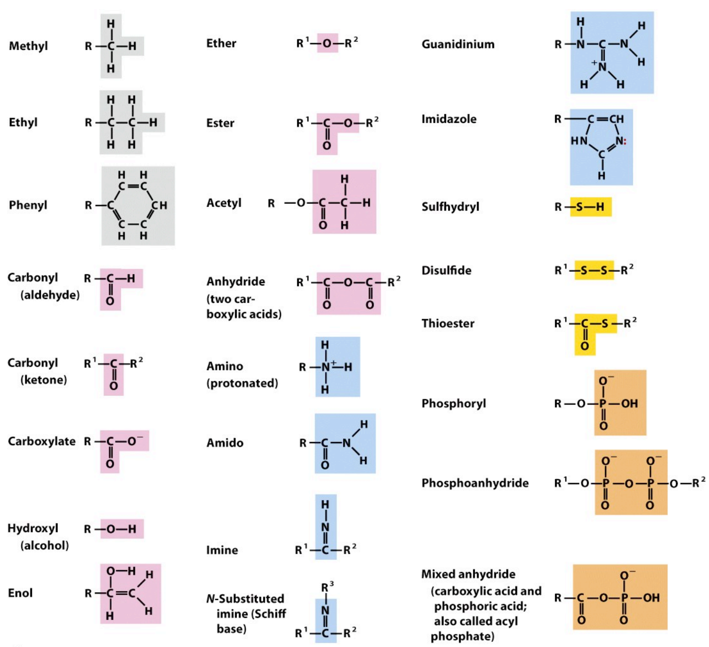


Figure 1-15
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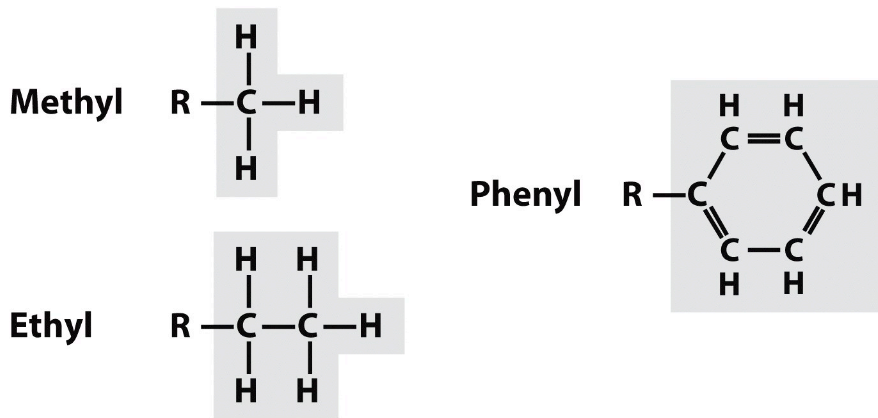

Figure 1-15 part 1
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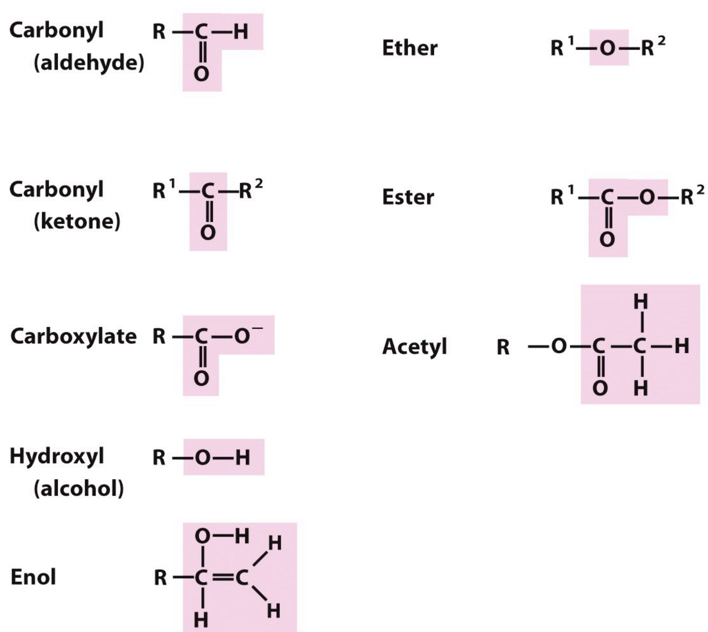

Figure 1-15 part 2
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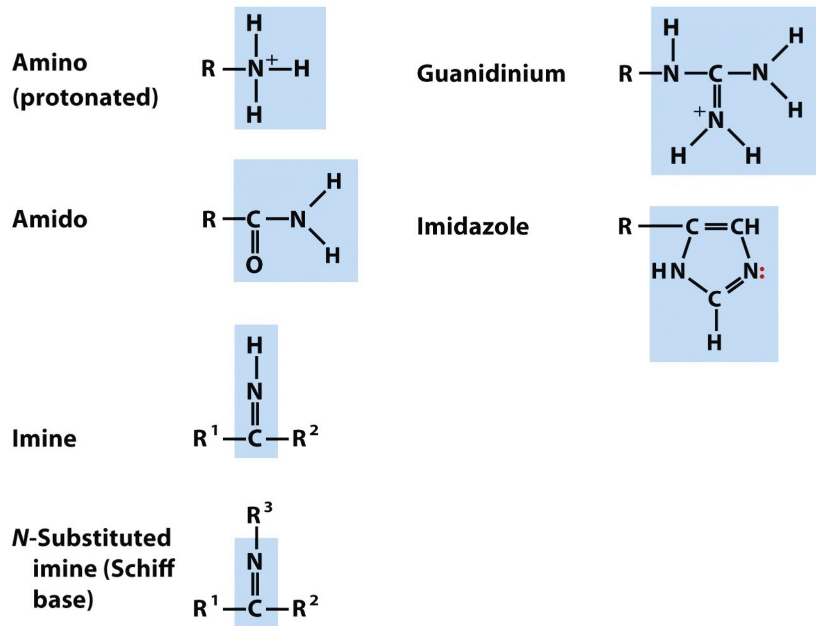

Figure 1-15 part 3
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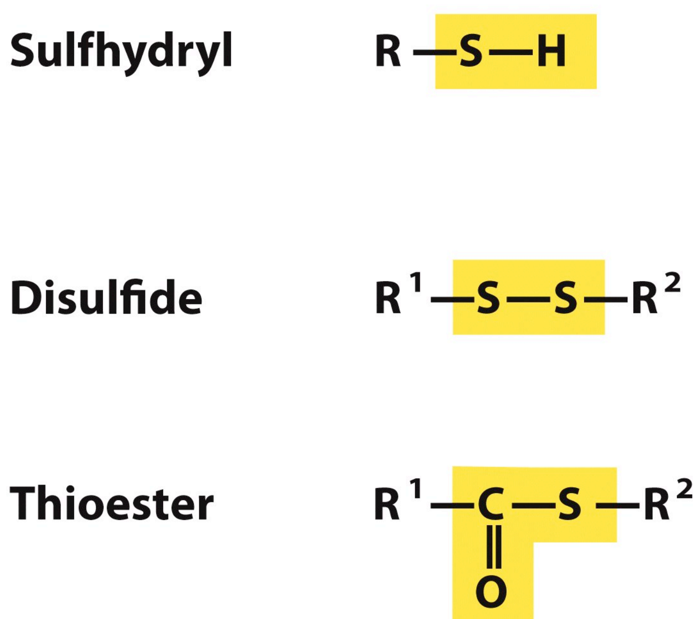

Figure 1-15 part 4
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Phosphoryl

Phosphoanhydride

Mixed anhydride (carboxylic acid and phosphoric acid; also called acyl phosphate)

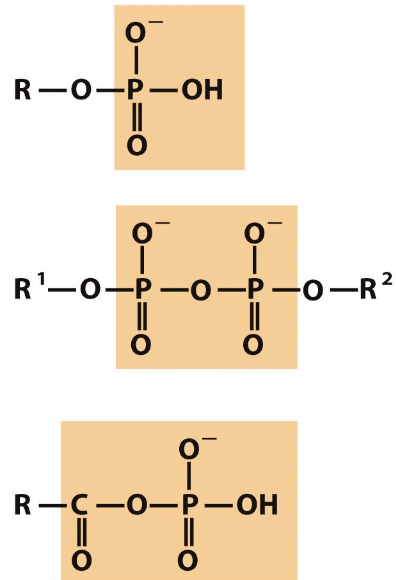

Figure 1-15 part 5
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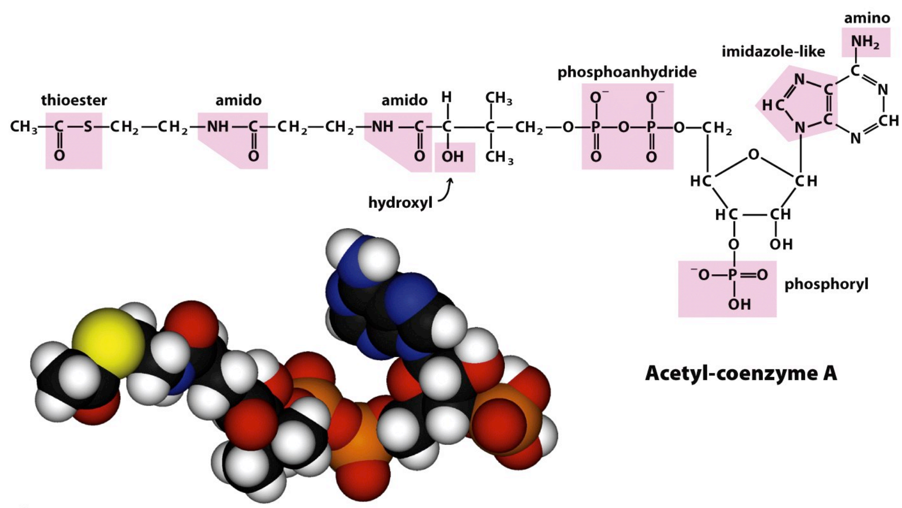

Acetyl-coenzyme A

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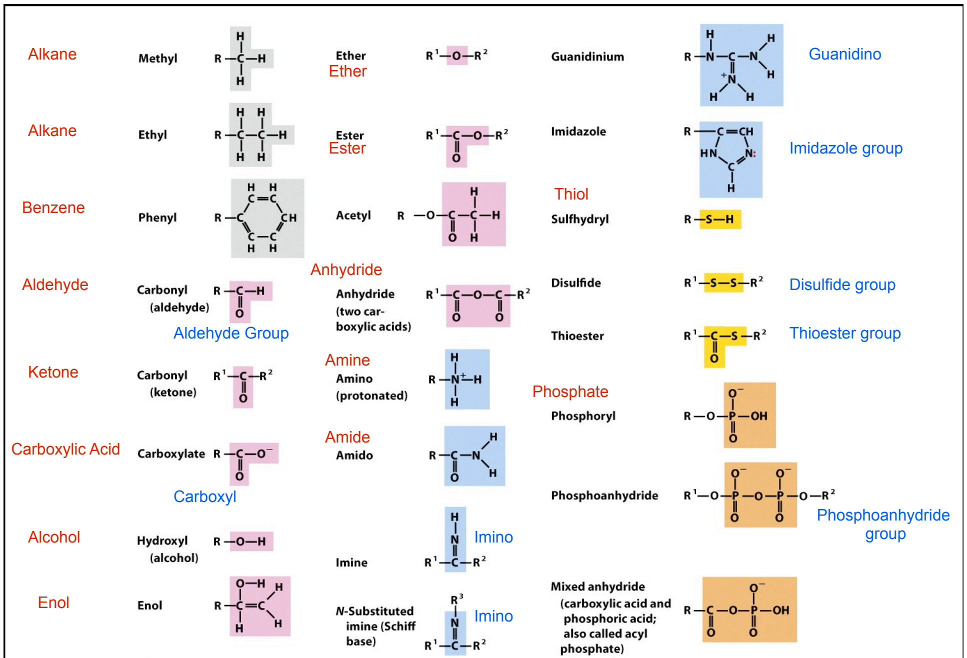

Figure 1-15
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TABLE 1–1 Molecular Components of an *E. coli* Cell

	Percentage of total weight of +1cell	Approximate number of different
Water	70	1
Proteins	15	3,000
Nucleic acids		
DNA	1	1
RNA	6	>3,000
Polysaccharides	3	5
Lipids	2	20
Monomeric subunits and intermediates	2	500
Inorganic ions	1	20

Table 1-1
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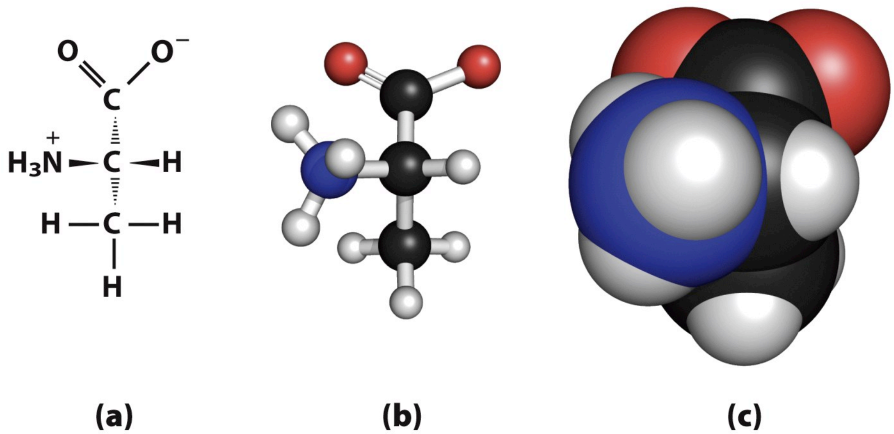

Figure 1-17
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functional group
Stereoisomers
cis-trans isomer or geometric isomers
chiral center
enantiomers
diastereomers
racemic mixtures
configuration
conformation
stereospecificity
dehydrogenations
nucleophiles
electrophiles
SN_1 & SN_2 substitution reaction

Type of Structural Isomers

1) Structural – Completely different structures

2) Geometric – Differ in Geometry – *cis* & *trans*

3) Stereo – Differ in their 3D – R & S

Cis-Trans Isomerism

Similar groups on same side of double bond, alkene is ***cis***.

Similar groups on opposite sides of double bond, alkene is ***trans***.

Cycloalkenes are assumed to be cis.

Trans cycloalkenes are not stable unless the ring has at least 8 carbons.

E-*Z* Nomenclature

Use the Cahn-Ingold-Prelog rules to assign priorities to groups attached to each carbon in the double bond.

If high priority groups are on the same side, the name is *Z* (for *zusammen*).

If high priority groups are on opposite sides, the name is *E* (for *entgegen*).

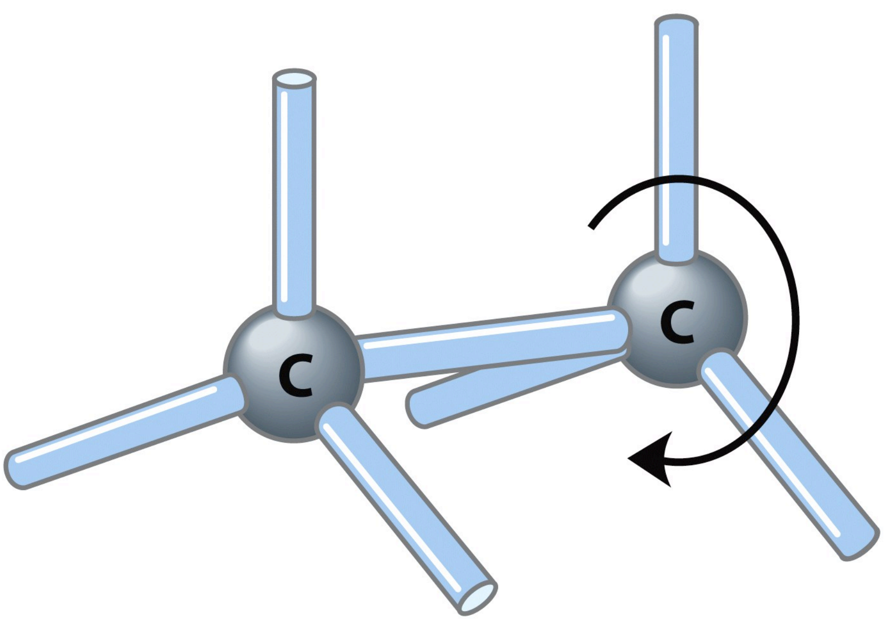

Figure 1-14b
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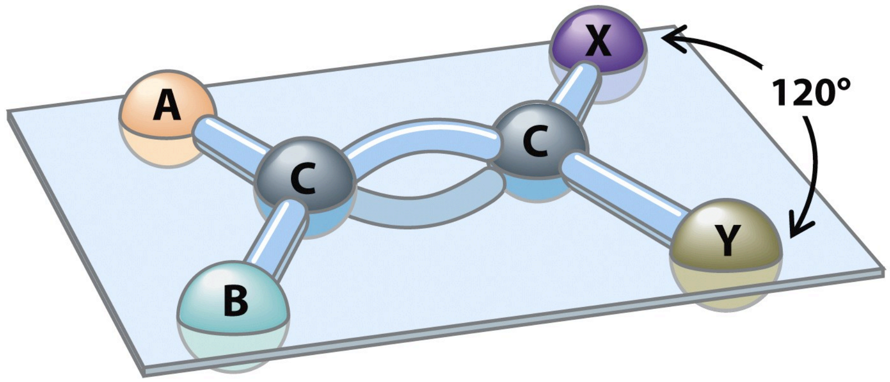

Figure 1-14c
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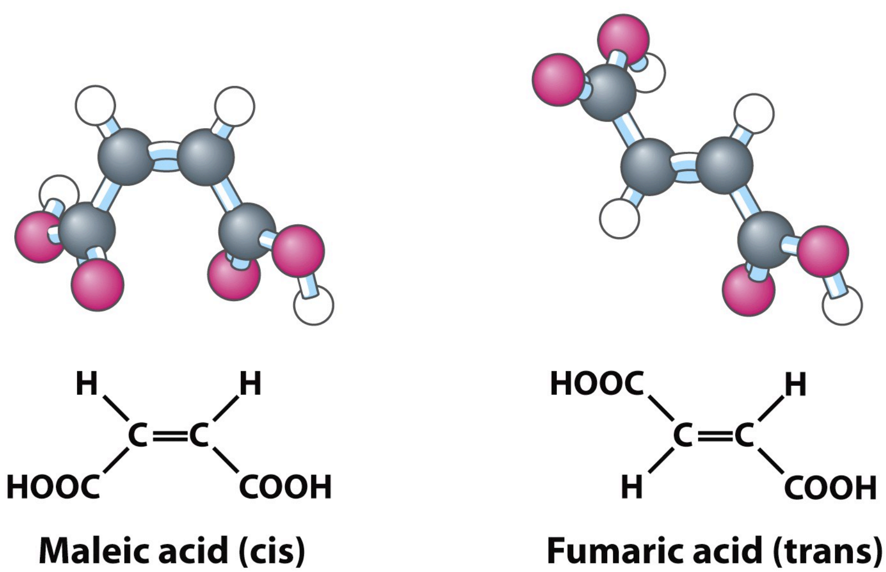

Figure 1-18a
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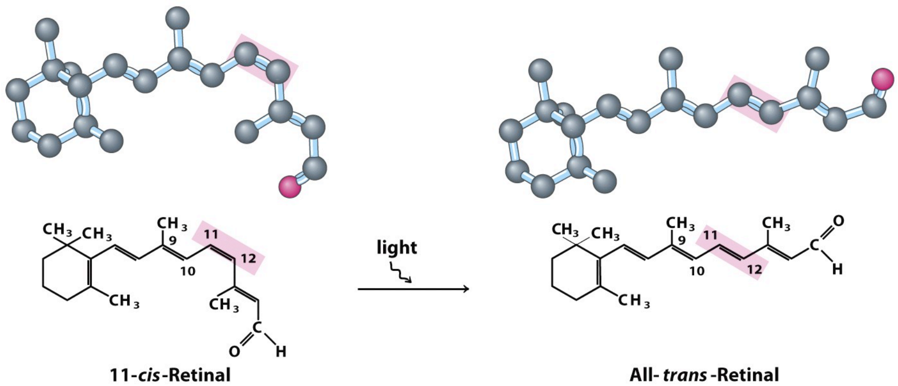

Figure 1-18b
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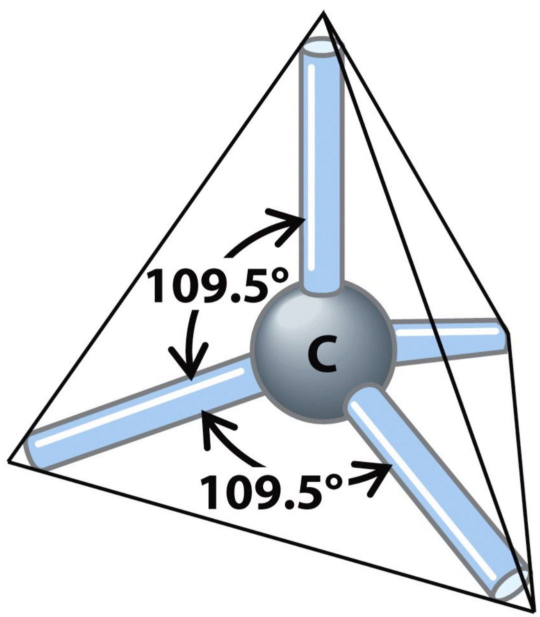

Figure 1-14a
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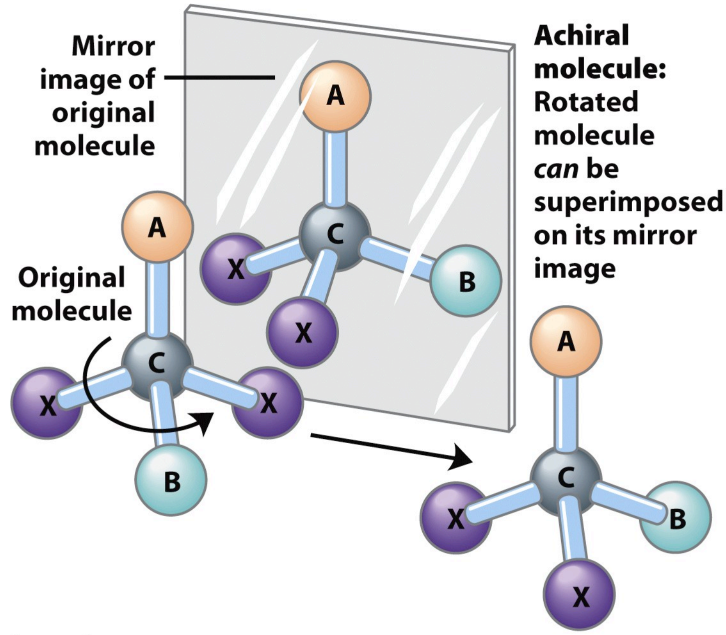

Figure 1-19b
Lehninger Principles of Biochemistry, Fifth Edition

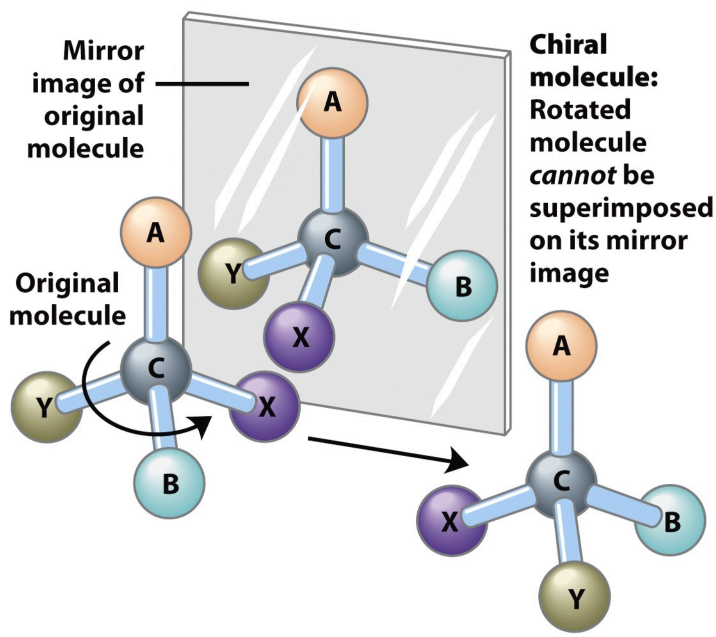

Figure 1-19a
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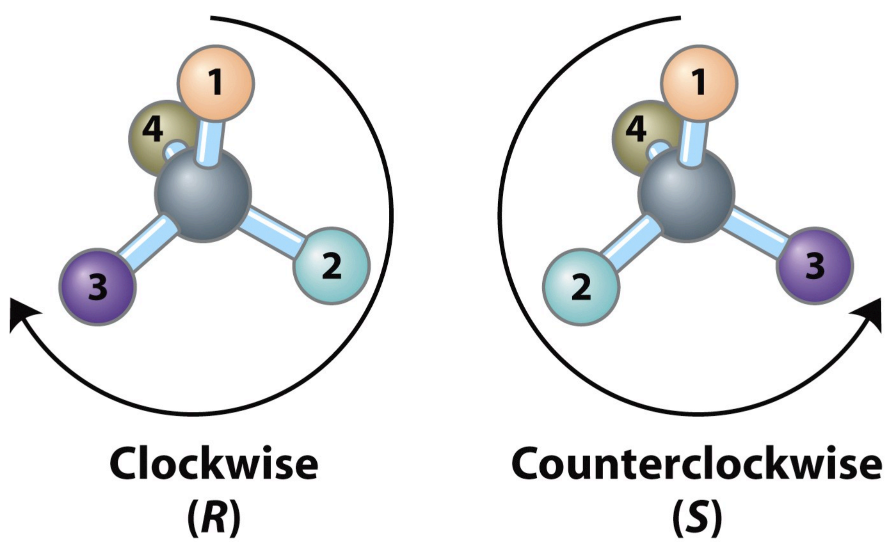
R & S Configuration

Arrange the smallest group in back, and put the other three groups in the order of large, medium and small. Move around these three groups, if clockwise, R configuration, however, if counter clockwise, then S configuration.

1. The larger the atomic number, the larger the group
2. For same atomic number, the large the atomic weight, the larger the group
3. If two groups with same atoms attach to the chiral center, then compare the atoms attaching to the two atoms adjacent to the chiral center.
4. Any double bond is considered as the equivalent of two single bond, for example, C=O is equivalent to two C-O bonds.



Unnumbered 1 p17a
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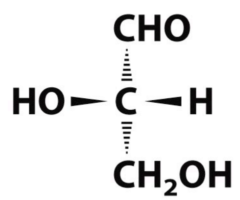
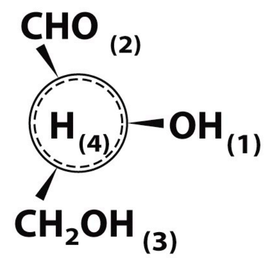


L-Glyceraldehyde



(*S*)-Glyceraldehyde

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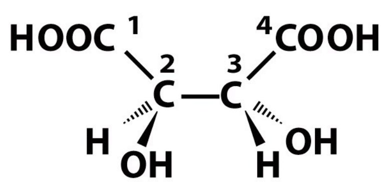
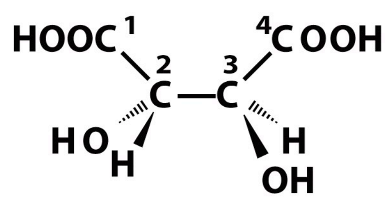


(2*R*,3*R*)-Tartaric acid (dextrorotatory)



(2*S*,3*S*)-Tartaric acid (levorotatory)

Box 1-2 figure 1
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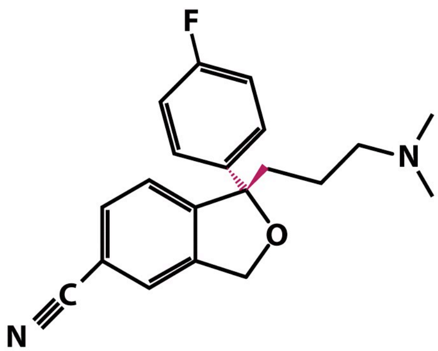
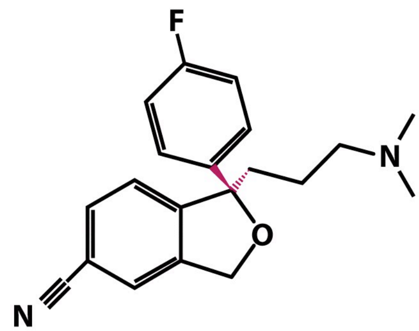


(*S*)-Citalopram



(*R*)-Citalopram

Figure 1-23c
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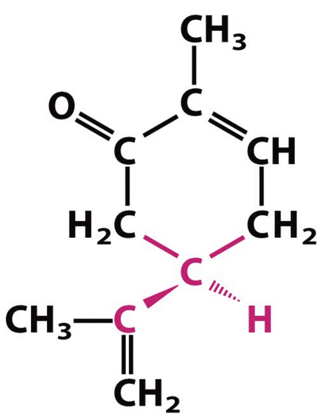
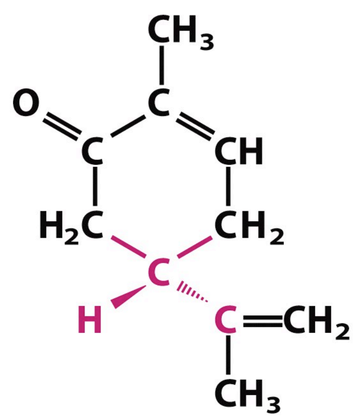


(*R*)-Carvone (spearmint)



(*S*)-Carvone (caraway)

Figure 1-23a
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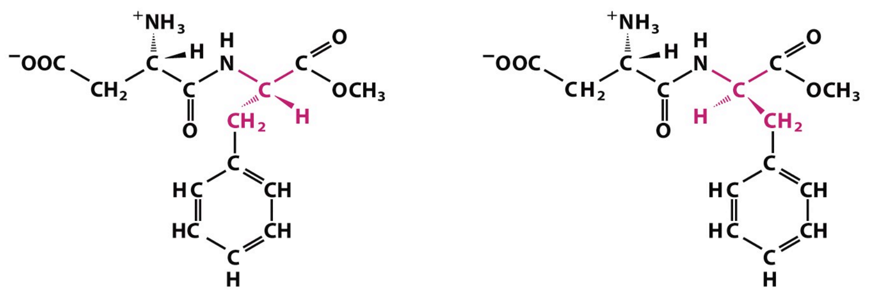

L-Aspartyl-L-phenylalanine methyl ester
(aspartame) (sweet)

L-Aspartyl-D-phenylalanine methyl ester
(bitter)

Figure 1-23b
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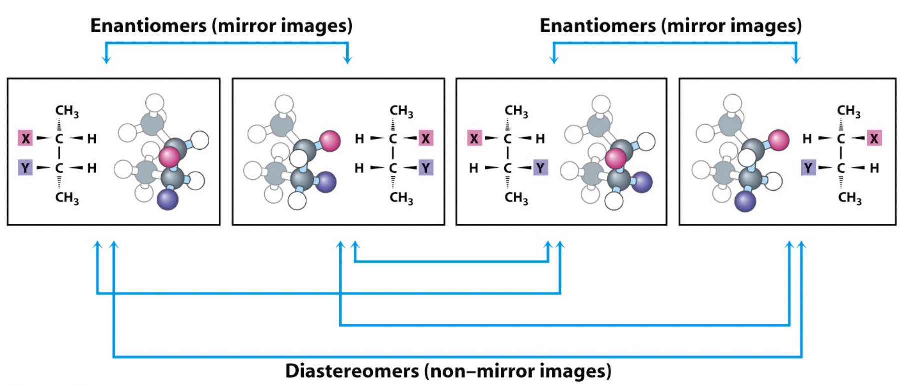

Figure 1-20
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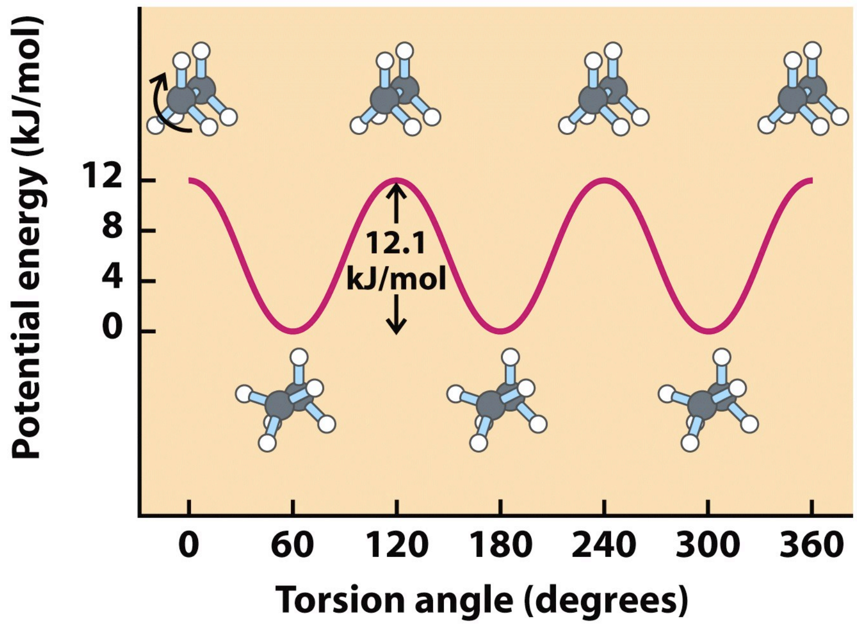

Figure 1-21
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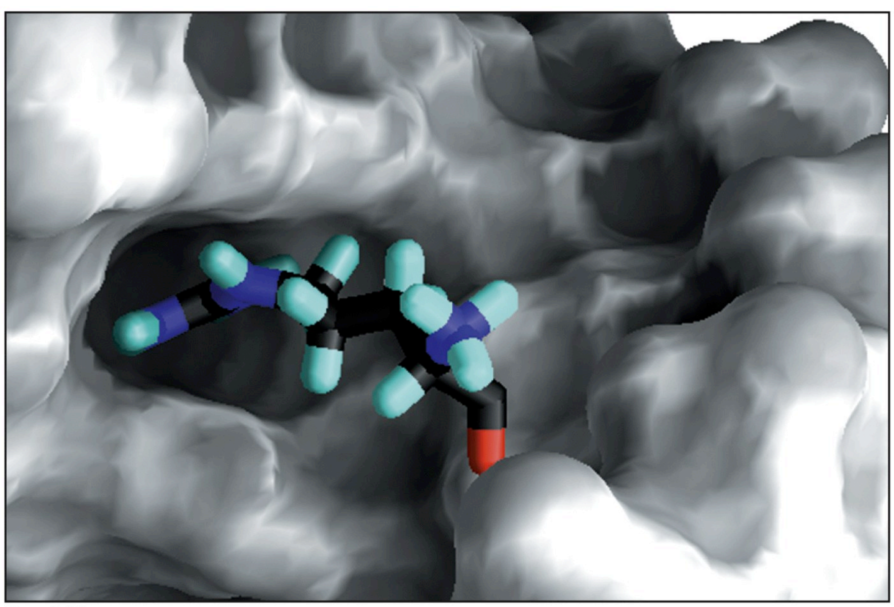

Figure 1-22
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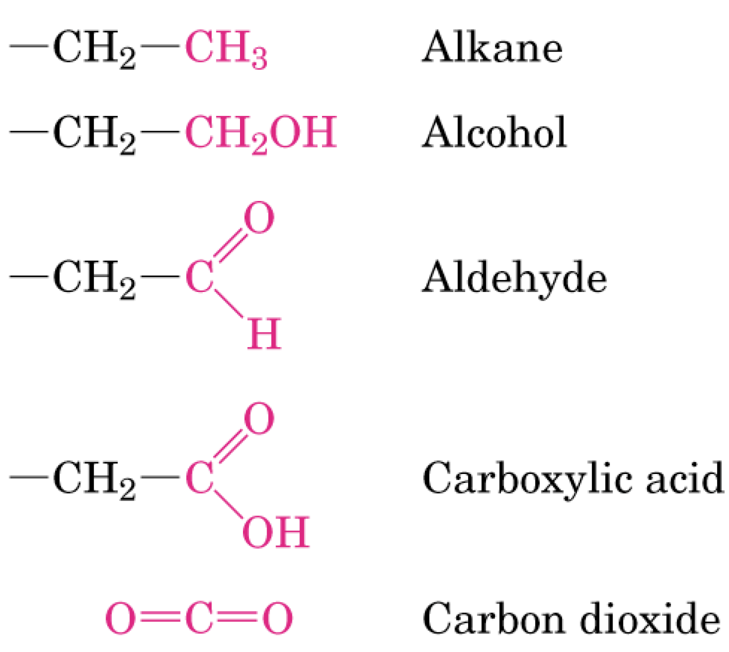
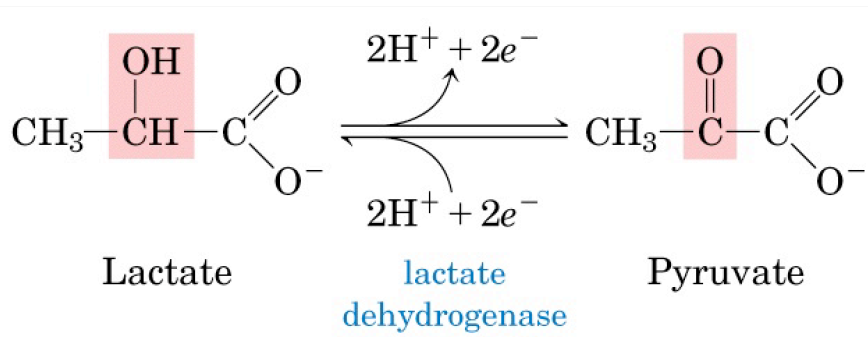
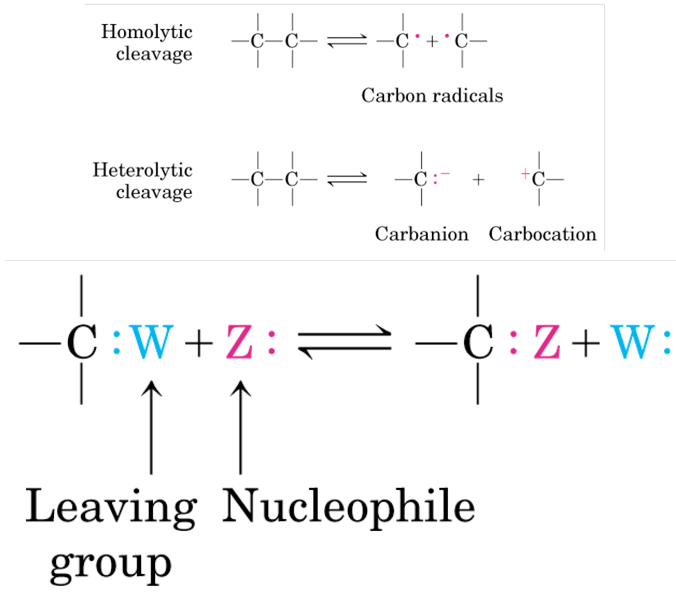
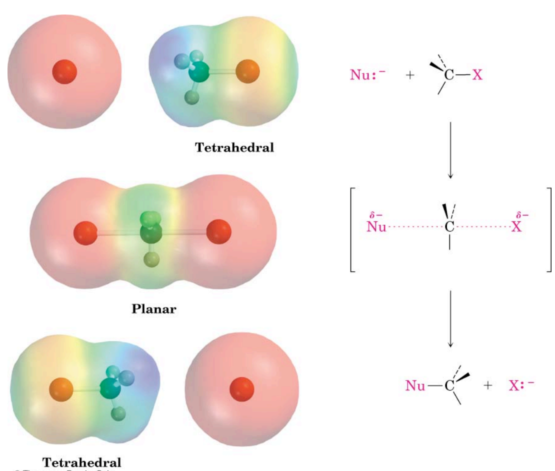


Oxidation- Reduction

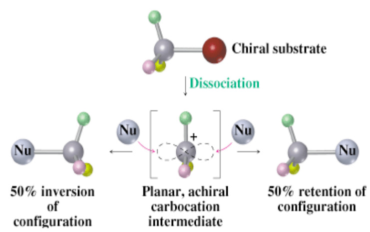


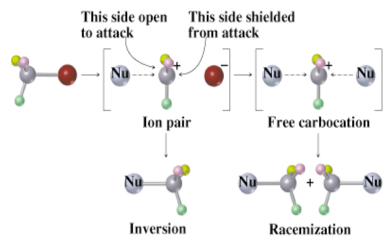


Mechanism of S_N2 Reaction

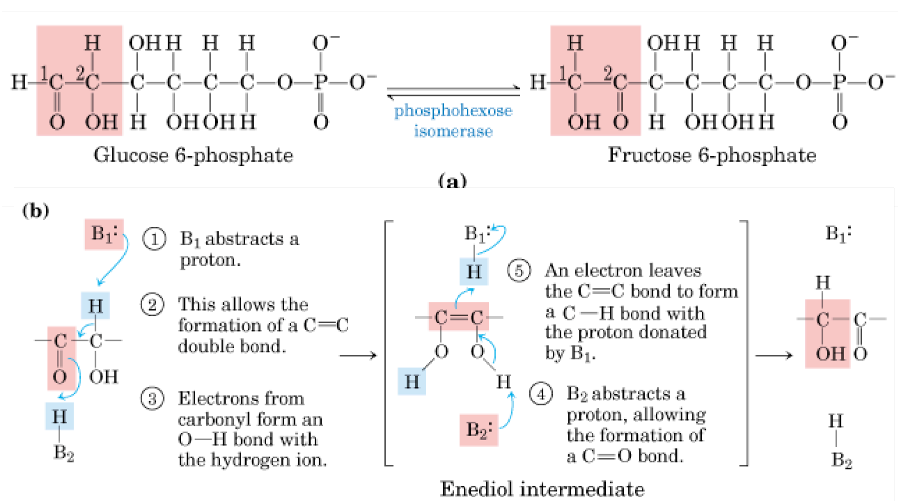


S_N1 Mechanism

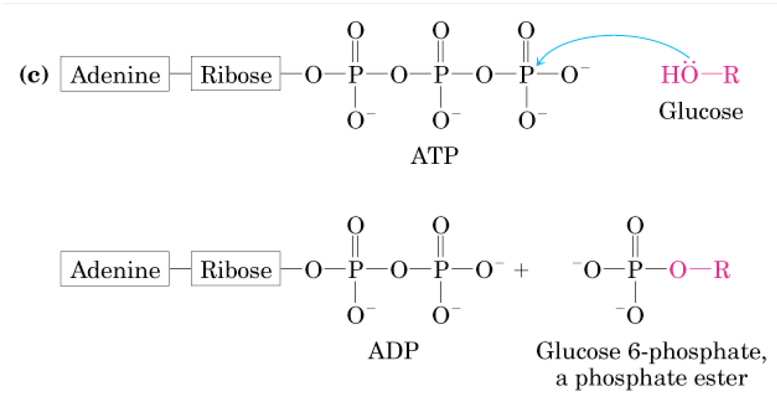




Internal Rearrangement



Group Transfer



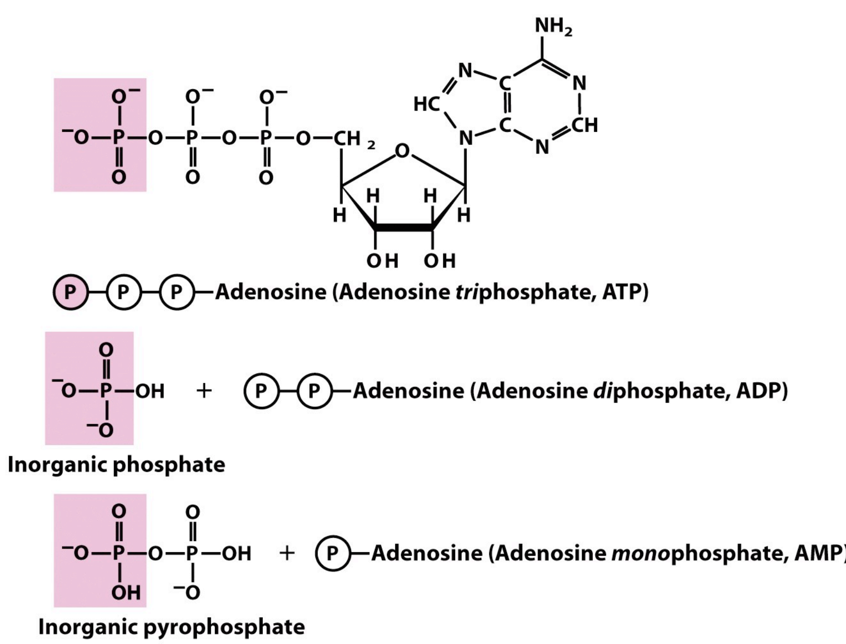


Figure 1-25
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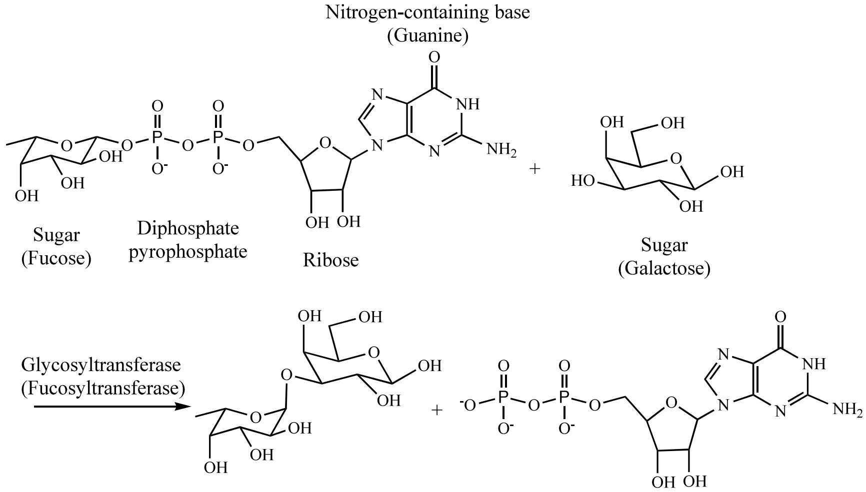

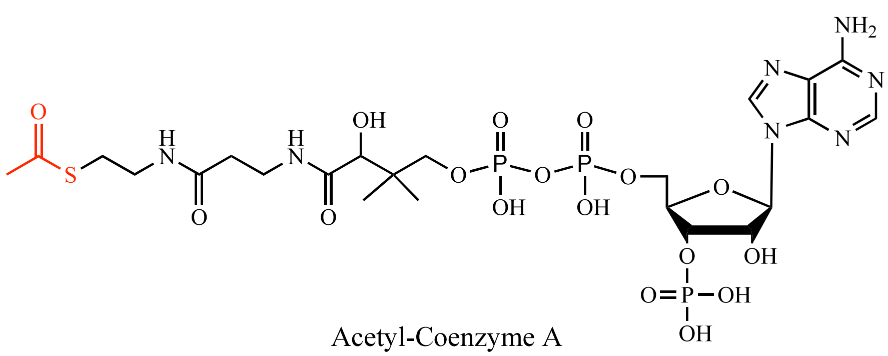

Acetyl-Coenzyme A
(Acetyl-CoA)

Condensation