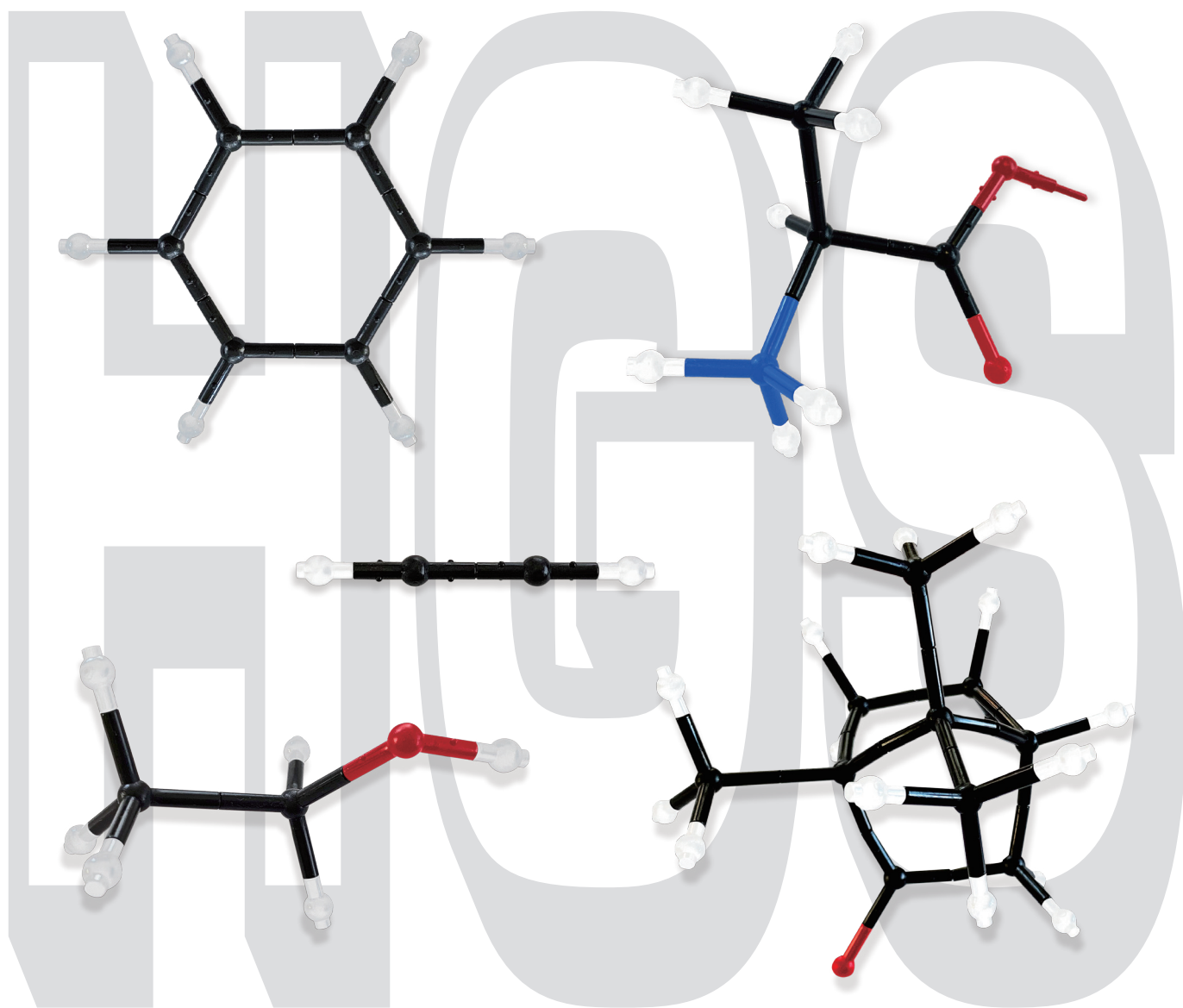


HGS

STEREOCHEMISTRY MOLECULAR MODEL

New Alpha Series Manual, 1st Edition

#4010 α Basic Set



MARUZEN

Tokyo, Japan

Contents

#4010 α Basic Set

Unassembled, 1 Å = 2.0 cm

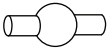
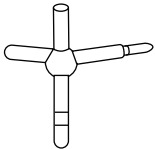
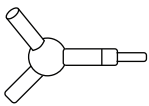

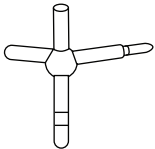
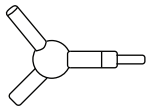
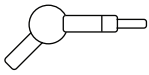

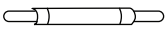

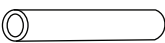
Item No.	Name	Shape	Color	Bond Radius	Bond Angle	Quantity
ORG-17	Hydrogen		white	0.33 Å		40
ORG-1	sp^3 Carbon		black	0.77 Å	109.47°	25
ORG-5	sp^2 Carbon		black	0.70 Å	120°	12
ORG-24	sp Carbon		black	0.60 Å	180°	2
ORG-2	sp^3 Nitrogen		blue	0.77 Å	109.47°	3
ORG-6	sp^2 Nitrogen		blue	0.70 Å	120°	2
ORG-12	Single bond Oxygen		red	0.66 Å	109.47°	8
ORG-15-1	Double bond Oxygen		red	0.62 Å		3
ORG-20	Connector		black			25
ORG-21	Double bond lock		transparent			3
ORG-22	Bond puller		black			1

Table 1. Bond length [\AA ($= 100 \text{ pm} = 10^{-10} \text{ m}$)] of common chemical bonds: "R" and "ar" indicate aliphatic and aromatic groups, respectively.

$(\text{sp}^3) \text{ C} - \text{C} (\text{sp}^3)$	1.54	$\text{C} = \text{O}$ (ester)	1.20
$(\text{sp}^3) \text{ C} - \text{C} (\text{sp}^2)$	1.51	$(\text{sp}^3) \text{ C} - \text{N} (\text{sp}^3)$	1.47
$(\text{sp}^3) \text{ C} - \text{C} (\text{sp})$	1.46	$(\text{sp}^2) \text{ C} = \text{N}$	1.28
$(\text{sp}^2) \text{ C} - \text{C} (\text{sp}^2)$	1.46	$(\text{sp}) \text{ C} \equiv \text{N}$	1.14
$(\text{ar}) \text{ C} - \text{C} (\text{ar})$	1.39	$(\text{sp}^3) \text{ C} - \text{S} (\text{sp}^3)$	1.82
$(\text{sp}^2) \text{ C} = \text{C} (\text{sp}^2)$	1.34	$(\text{sp}^2) \text{ C} = \text{S}$	1.67
$(\text{sp}) \text{ C} \equiv \text{C} (\text{sp})$	1.20	$(\text{sp}^3) \text{ C} - \text{P} (\text{sp}^3)$	1.86
$(\text{sp}^3) \text{ C} - \text{H}$	1.09	$(\text{sp}^3) \text{ C} - \text{Si} (\text{sp}^3)$	1.86
$(\text{sp}^2) \text{ C} - \text{H}$	1.08	$(\text{sp}^3) \text{ C} - \text{F}$	1.40
$(\text{sp}^3) \text{ C} - \text{OH}$	1.43	$(\text{sp}^3) \text{ C} - \text{Cl}$	1.80
$\text{RC}(=\text{O}) - \text{OR}$	1.34	$(\text{sp}^3) \text{ C} - \text{Br}$	1.97
$\text{RC}(=\text{O}) - \text{OH}$	1.31	$(\text{sp}^3) \text{ C} - \text{I}$	2.14
$\text{RC}(=\text{O})\text{O} - \text{R}$	1.44	$\text{O} - \text{H}$ (alcohol)	0.97
$\text{R} - \text{OR}$	1.43	$\text{O} - \text{H}$ (acid)	1.02
$(\text{ar}) \text{ C} - \text{OR}$	1.36	$\text{N} - \text{H}$ (amine)	1.01
$\text{C} = \text{O}$ (ketone)	1.21	$\text{N} = \text{O}$ (nitro)	1.22

1. Nature of Chemical Bond: the Concept of Covalent Bond based on Quantum Mechanics

It is well known that in the beginning of the 20th century, the nature of chemical bond was clarified by introducing the concept of a covalent bond based on quantum mechanics. Before quantum mechanics, i.e., at the time of classical mechanics, it was difficult to explain the reason why two neutral hydrogen atoms combine with each other to generate a H_2 molecule. Based on quantum mechanics, the $1s$ atomic orbital of a hydrogen atom interacts with that of the other hydrogen atom to generate a σ orbital with bonding nature and a σ^* orbital with anti-bonding nature (Figure 1 (a)). The two electrons occupy the lower energy σ orbital to release binding energy; thus, the H_2 molecule is stabilized. The two electrons that combine two hydrogen nuclei are called shared electrons. This is the concept of a covalent bond. Figure 1 (b) depicts a model of a H_2 molecule constructed with HGS Stereochemistry Molecular Models.

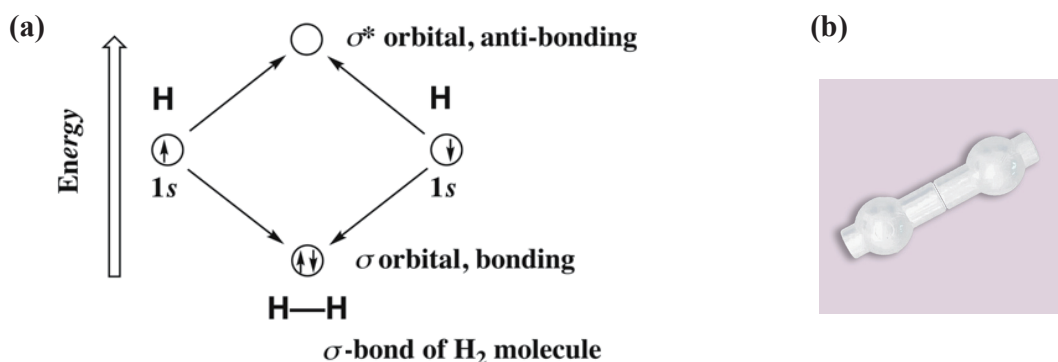


Figure 1
A diagram showing σ -bond formation in the H_2 molecule.

2. Atomic and Molecular Structures: Hybrid Orbitals, Bond Angle, and Bond Length

The concepts of covalent bonds and hybrid orbitals are very important for understanding bonds between atoms and hence molecular structures. For example, in the case of a methane molecule, the $2s$, $2p_x$, $2p_y$, and $2p_z$ atomic orbitals of the central carbon atom make four sp^3 hybrid orbitals, which form a tetrahedral configuration as shown in Figure 2 (a). An unpaired electron in each sp^3 hybrid orbital makes a covalent bond with the $1s$ electron of a hydrogen atom. Therefore, the carbon atom binds with four hydrogen atoms to make a methane molecule, which has a symmetrical tetrahedral structure as depicted in Figure 2.

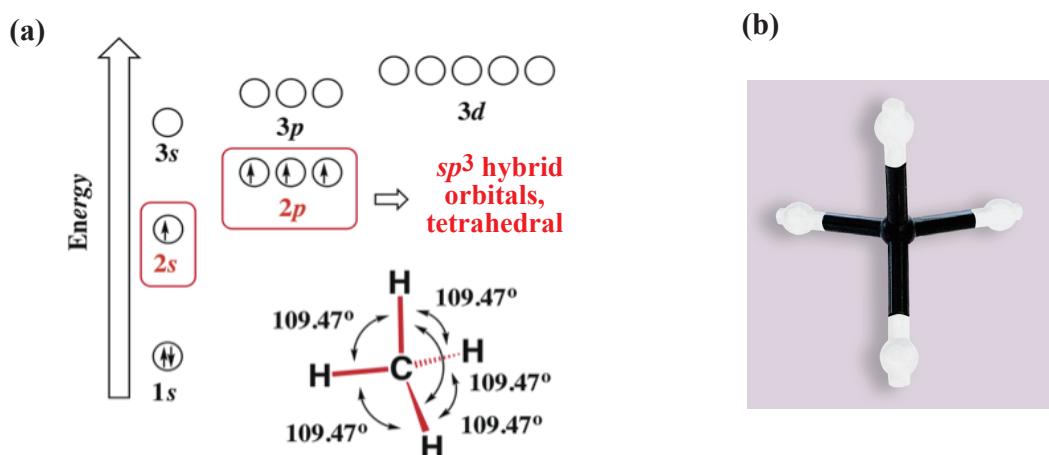


Figure 2

The atomic orbitals and energy levels of an alkane carbon atom, from which four new sp^3 hybrid orbitals (red color) are formed taking a tetrahedral structure as exemplified by a methane molecule. All bond angles H-C-H are 109.47° .

Figure 2 (b) depicts the molecular model of methane constructed with the present HGS Stereochemistry Molecular Models. In the present stereochemistry models, the bonds and atom unite with each other as shown; namely the bonds and atom are not separable. In the case of the central sp^3 carbon atom (ORG-1), the four bonds are oriented to make a regular tetrahedron. Therefore, all bond angles are 109.47° .

The construction of a methane molecule is illustrated in Figure 3. For connecting ORG-17 hydrogen atom to the bond (hole) of sp^3 carbon atom, ORG-20 connector is used as shown.

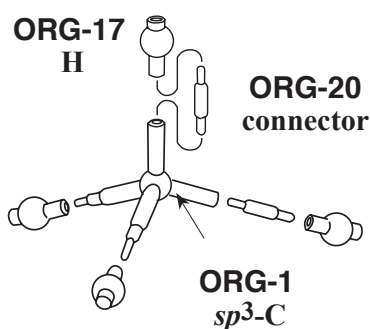


Figure 3

The construction of methane model: when necessary, an ORG-20 connector is used.

In HGS Stereochemistry Molecular Models, the scale is $1 \text{ \AA} = 2.0 \text{ cm}$. Therefore, it is easy to estimate the interatomic distance by using a ruler. For instance, the C-H bond length in the model is ca. $2.20 \text{ cm} = 1.10 \text{ \AA}$: the actual C-H distance of aliphatic hydrocarbons experimentally determined is 1.09 \AA (see Table 1). Thus, the present stereochemistry model is useful also for estimating interatomic distances.

3. Alkanes, Saturated Hydrocarbons, and Conformational Change

An ethane molecule is made of two sp^3 carbon atoms (ORG-1) and six hydrogen atoms (ORG-17) as depicted in Figure 4, where two conformers are shown: (a) staggered conformation and (b) eclipsed conformation.

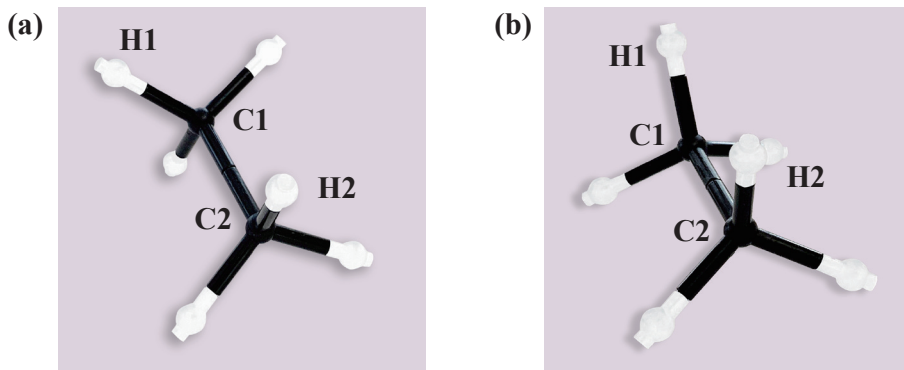


Figure 4

**The two conformers of ethane molecule:
(a) staggered conformation, (b) eclipsed conformation.**

In the staggered conformation, the dihedral angle H1-C1-C2-H2 is 60° , while in the eclipsed conformation, the dihedral angle H1-C1-C2-H2 is 0° . The models point out the fact that the staggered conformer is more stable than the eclipsed one. Why would this be the case? Because in the eclipsed conformation, the electrons in the two C-H σ -bonds, i.e., C1-H1 and C2-H2 bonds, are close to one another, and hence the conformer becomes less stable due to the electronic repulsion. On the other hand, in the staggered conformation, the electrons in the two C-H σ -bonds, i.e., C1-H1 and C2-H2 bonds, are more remote, and therefore, the staggered conformation is the most stable one. In most molecules, the staggered conformations are more stable.

In the model of ethane, the distance between two carbon atoms is measured to be ca. $3.10 \text{ \AA} = 1.55 \text{ \AA}$, which is comparable to the actual $C(sp^3)-C(sp^3)$ bond length, 1.54 \AA , of regular hydrocarbons that has been determined experimentally (Table 1).

Figure 5 depicts two conformers of cyclohexane, i.e., chair form and boat form. As you may know, the chair form is more stable than the boat form. Why is this true? Because in the boat form, the moiety C1-C2-C3-C4 takes an eclipsed conformation as shown. In addition, all hydrogen atoms attached to C2 and C3 also take eclipsed conformations. The same is true for the C4-C5-C6-C1 moiety. Therefore, the boat conformer becomes less stable.

On the other hand, in the chair form of cyclohexane, all moieties take staggered conformations: there is no eclipsed interaction at all. Therefore, it is the most stable conformer.

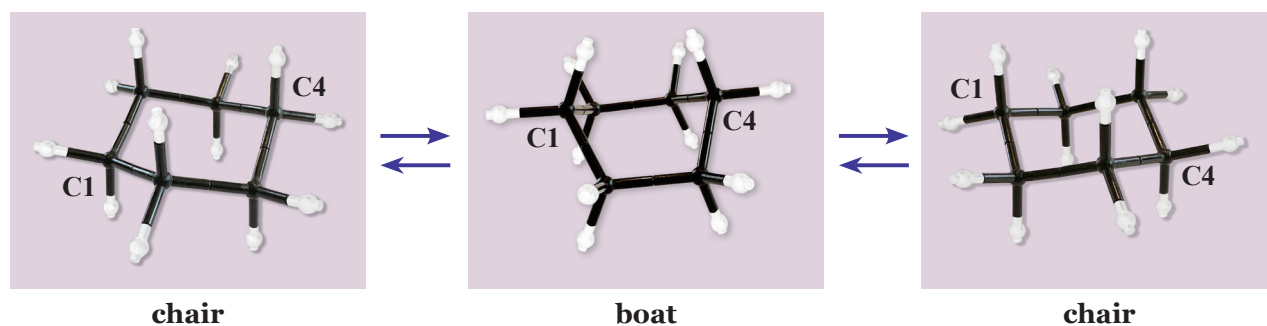


Figure 5

The models of cyclohexane: the ring flip between two stable chair conformers via the intermediate of boat conformer.

Figure 5 shows the ring flip of cyclohexane ring also. Namely, the chair conformer undergoes the ring flip to form the other chair form, via the intermediate of boat form.¹ The HGS Stereochemistry Model is very useful for demonstrating the ring flip, because the partial rotation around the C-C bond is smooth during the conformational changes.

¹ The details of the cyclohexane ring flip are more complex, because the energy calculation indicated that the twist-boat form is an energy minimum in the course of the ring flip of chair form; the boat form is not an energy minimum. However, the details are beyond the discussion here using molecular models.

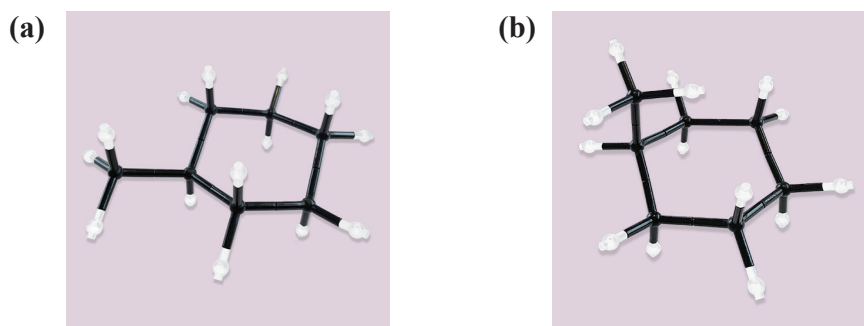


Figure 6

Two conformers of methylcyclohexane: (a) the form with an equatorial methyl group; (b) the form with an axial methyl group.

Figure 6 depicts the two conformers of methylcyclohexane: (a) the form with an equatorial methyl group; (b) the form with an axial methyl group. Thus, this molecular model is very useful for showing the equatorial and axial orientations. It is known that the equatorial conformer is more stable than the axial one, because in the axial form, the repulsion between the axial methyl group and two axial protons makes the conformer to be less stable. Such a repulsion is called a 1,3-diaxial interaction.

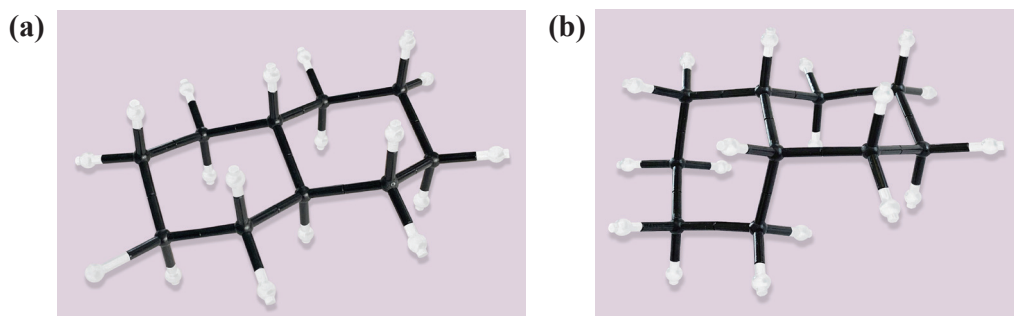


Figure 7
The structures of (a) *trans*-decalin and (b) *cis*-decalin.

As bicyclic compounds, the models of *trans*-decalin and *cis*-decalin are depicted in Figure 7. In model (a), since the two protons at the ring junction are *trans*, it is called *trans*-decalin. On the other hand, in model (b), the two protons are *cis*, and hence it is named *cis*-decalin. Thus, these compounds are stereoisomers of each other.

4. Alkenes and Aromatic Compounds

In the case of alkane molecules discussed above, the carbon atoms take tetrahedral configurations with sp^3 hybrid orbitals.

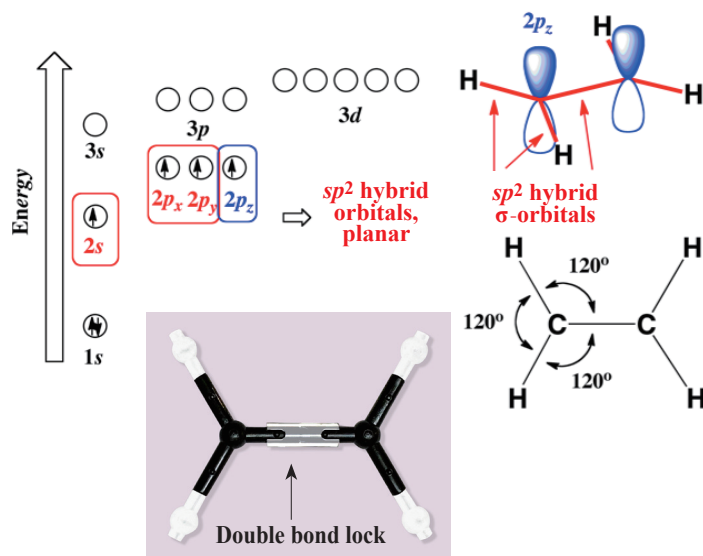


Figure 8
The atomic orbitals and energy levels of an alkene carbon atom, from which three new sp^2 hybrid orbitals (red color) are formed taking a trigonal planar structure as exemplified by an ethylene molecule. All bond angles are 120° .

On the other hand, a carbon atom can take another configuration, i.e., a planar configuration with sp^2 hybrid orbitals, which are made of $2s$, $2p_x$, and $2p_y$ atomic orbitals as shown in the case of ethylene molecule (Figure 8).

The remaining $2p_z$ atomic orbital is used to form a π -bond with the $2p_z$ orbital of the next carbon atom. These two $2p_z$ orbitals are parallel to each other, because of the stabilization by the maximum overlap of π -atomic orbitals. As a consequence, all of the atoms of ethylene molecule lie in a single plane. Although the model of ethylene can rotate around the C-C σ -bond, it is possible to block the rotation by using the part ORG-21, double bond lock, as shown in Figure 8.

The C=C length in the model is $2.80 \text{ cm} = 1.40 \text{ \AA}$, which is a little longer than the experimental bond length of $C(sp^2)=C(sp^2)$, 1.34 \AA (Table 1).

Figure 9 depicts the stable half-chair conformation of cyclohexene, where C6-C1-C2-C3 atoms lie in a single plane.

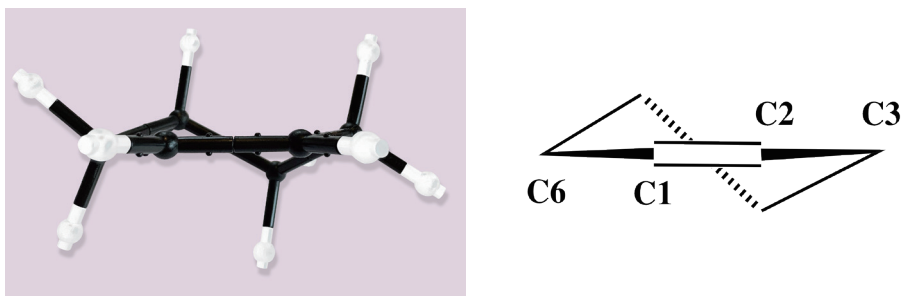


Figure 9

The side view of cyclohexene taking the half-chair conformation, where C6-C1-C2-C3 atoms lie in a single plane.

It is easy to make aromatic ring compounds by using the present models. Figure 10 shows a model of benzene, where the C-C length in the model is $2.80 \text{ cm} = 1.40 \text{ \AA}$, which is comparable to the experimental bond length of $C(\text{arom})-C(\text{arom})$, 1.39 \AA (Table 1).

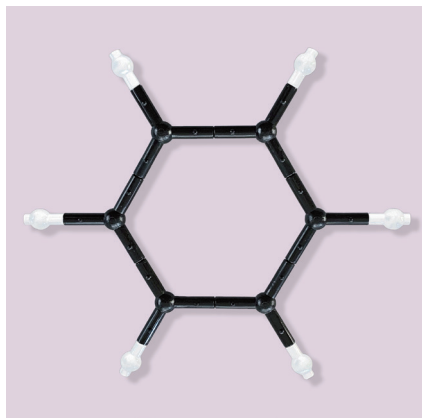


Figure 10

A model of benzene.

5. Acetylene and Alkyne Compounds

A carbon atom in alkyne compounds takes a linear configuration based on sp hybrid orbitals as exemplified by the case of acetylene molecule (Figure 11). Namely, the $2s$ and $2p_x$ atomic orbitals of a carbon atom make two sp hybrid orbitals, and the bond angle between them is 180° . The remaining $2p_y$ and $2p_z$ orbitals are used as π -bonds as shown.

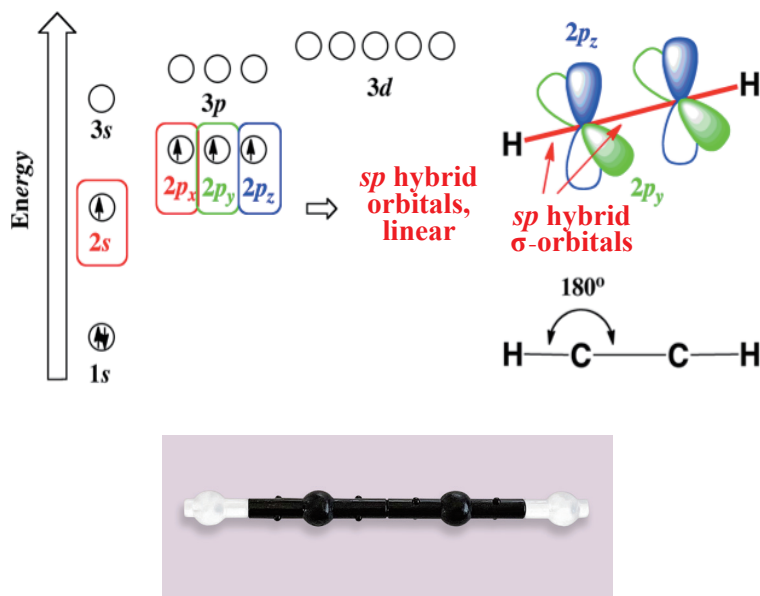


Figure 11

The atomic orbitals and energy levels of an alkyne carbon atom, from which two new sp hybrid orbitals (red color) are formed taking a linear structure as exemplified by an acetylene molecule: bond angle is 180° . The remaining $2p_y$ and $2p_z$ orbitals are used for π -bonds.

The model of acetylene molecule is shown in Figure 11, where two ORG-24 sp carbon atoms are connected to each other. The distance between two carbon atoms is $2.40 \text{ cm} = 1.20 \text{ \AA}$, which is comparable to the actual triple bond length 1.18 \AA (Table 1).

The Stereochemistry Model set is useful for constructing other alkyne compounds.

6. Alcohols, Ethers, Ketones, and Esters

Next, let's construct models of alcohols, ethers, ketones, and esters. As a typical example of an alcohol, a model of ethanol is shown in Figure 12 (a), where ORG-12 is used as a single bond oxygen atom having an sp^3 configuration. Therefore, the bond angle C-O-H is 109.47° .

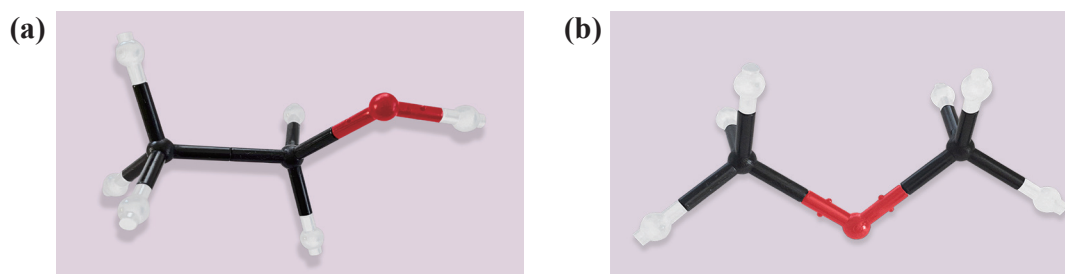


Figure 12
Models: (a) ethanol; (b) dimethyl ether.

The distance between C-O atoms in the ethanol model is 1.43 \AA , which is equal to the averaged experimental bond length 1.43 \AA (Table 1). In addition, the distance between O-H atoms is 0.99 \AA , which is comparable to the averaged experimental value 0.97 \AA (Table 1).

A model of dimethyl ether is shown in Figure 12 (b). The bond angles and lengths are similar to those of ethanol.

Figure 13 depicts the models of (a) acetone and (b) ethyl acetate. In the case of acetone, ORG-5 (sp^2 -C) and ORG-15-1 (double bond O) are used to form a carbonyl group. The distance of the C=O bond is 1.32 \AA , which is a little longer than the averaged experimental bond length 1.21 \AA (Table 1).

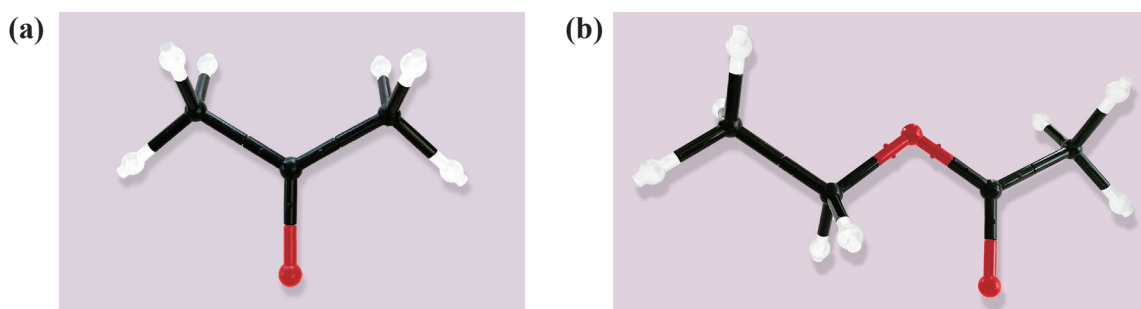


Figure 13
Models: (a) acetone; (b) ethyl acetate.

Similarly, a model of ethyl acetate is constructed as shown in Figure 13 (b), where the distance between ORG-12 (single bond O) and ORG-5 (sp^2 -C) is 1.36 Å, which is comparable to the averaged experimental bond length 1.34 Å (Table 1).

The present Stereochemistry Molecular Model set is useful for constructing more complex molecules. For example, Figure 14 depicts the model of (1*R*,4*R*)-(+)-camphor, a natural product isolated from camphor trees. As will be discussed later, the stereochemistry model is useful for recognizing the absolute configuration of such a little complex compound.

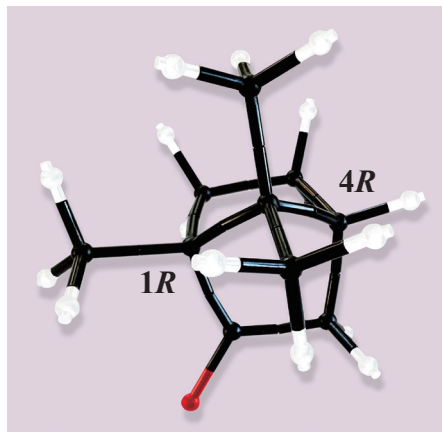


Figure 14
A model of (1*R*,4*R*)-(+)-camphor.

7. Amines, Amides, and Amino acids

The present stereochemistry model set contains the parts ORG-2 (sp^3 -N) and ORG-6 (sp^2 -N), which are useful for constructing amine and amide compounds, as exemplified in Figure 15.

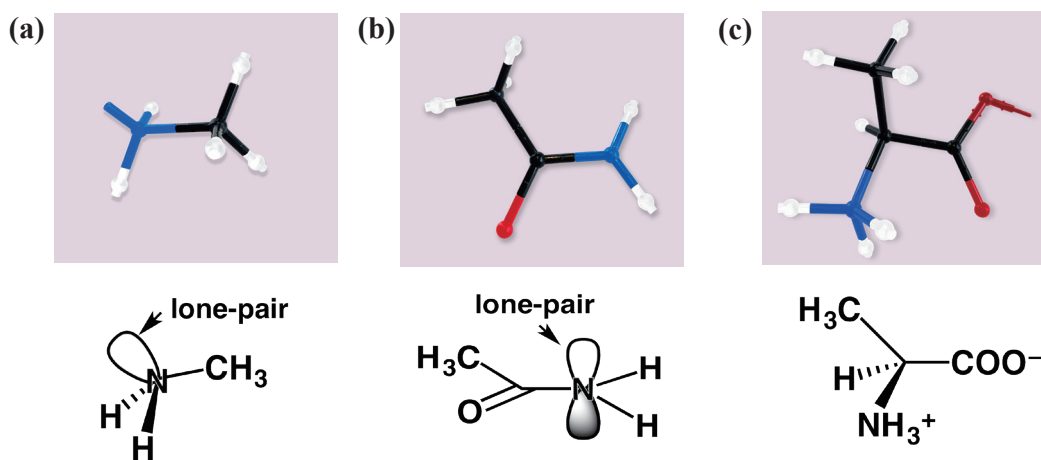


Figure 15
Models and stereo-structures of nitrogen compounds:
(a) methylamine; (b) acetamide; (c) *L*-alanine.

In the case of methylamine, the nitrogen atom takes the sp^3 configuration (ORG-2), where one hybrid orbital is used for the lone-pair electrons as shown in (a). On the other hand, the nitrogen atom of acetamide takes an sp^2 configuration (ORG-6) as illustrated in (b), because the lone-pair electrons are withdrawn by the adjacent C=O group, and hence to conjugate with the π -orbital of carbonyl group. Thus, the lone-pair orbital also takes the form of π -orbital to make the conjugation.

Figure 15 (c) depicts the model of *L*-alanine, where the amino group is protonated to form -NH_3^+ , while the carboxyl group shows the deprotonated anion form -COO^- . This is a typical example of the zwitter ion form of amino acids.

8. Absolute Configurations of Chiral Compounds

It is well known that three-dimensional compounds can take two structures, i.e., the original one and the mirror-imaged structure. If the two structures cannot be overlapped at all, these compounds are chiral. For example, natural amino acids have the chiral structures of *L*-absolute configuration as exemplified in Figure 16.

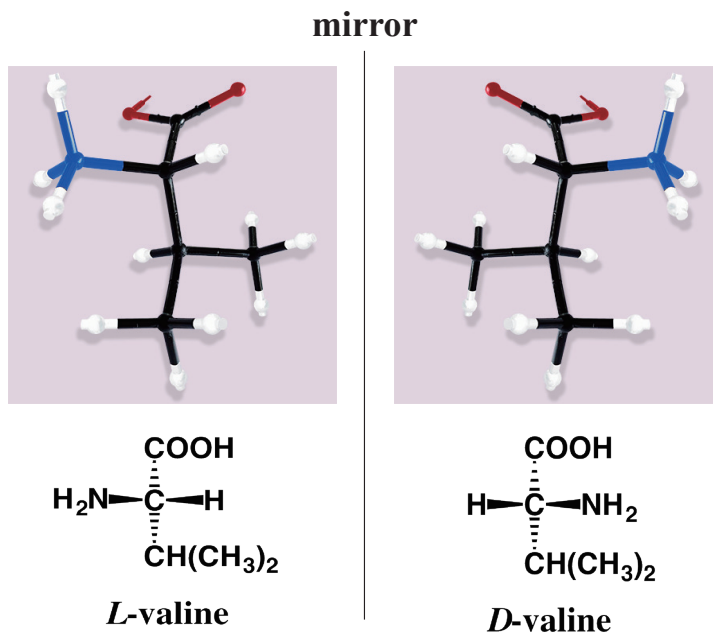


Figure 16

The models and mirror image structures of valine. In *L*-valine, the amino group locates on the left side, while in *D*-valine, it locates on the right side.

As shown in the lower part of Figure 16, the carboxyl group is placed at the top and rear, while the amino acid side chain, i.e., $\text{CH}(\text{CH}_3)_2$ here, is placed at the bottom and rear. If the amino group locates on the left and front side, it is defined as the *L*-absolute configuration. If on the right and front side, it is the *D*-configuration. This definition is applicable to all α -amino acids. So, the present molecular model is useful to study the definition.

On the other hand, for most organic compounds, another definition using *R* (right) and *S* (left) symbols is used as exemplified in Figure 17.

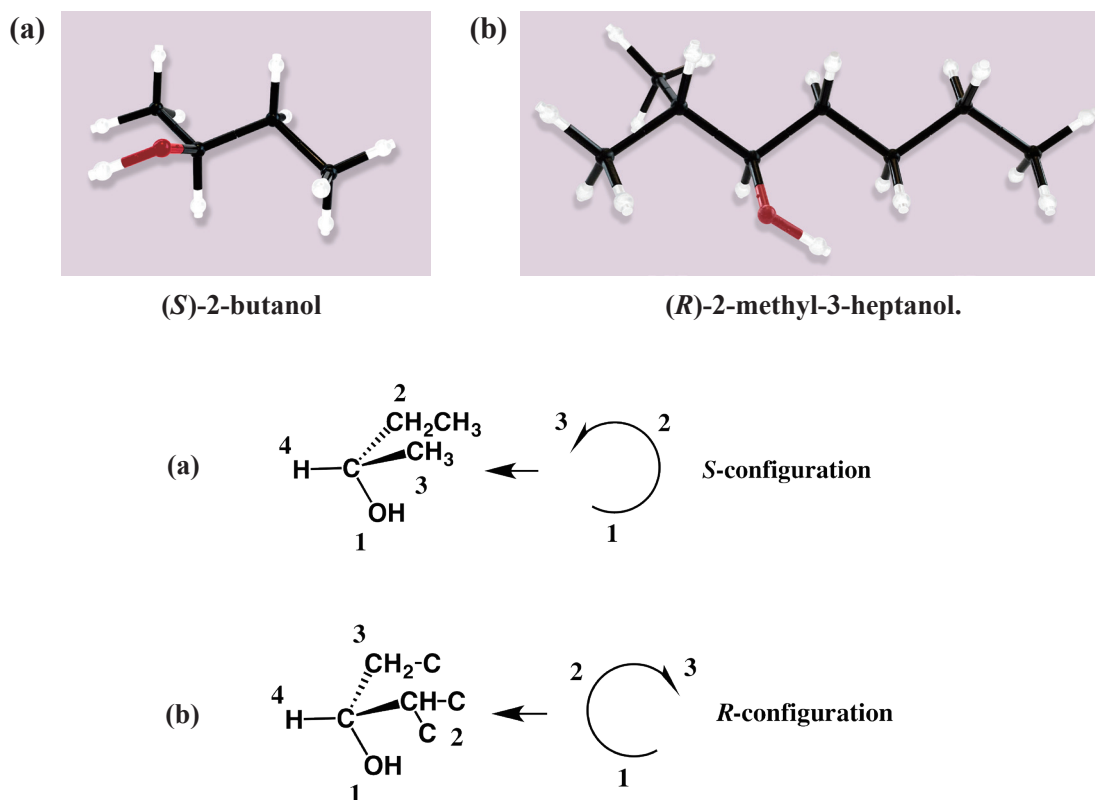


Figure 17

The models of chiral alcohols and the definition of (*R*)- and (*S*)-absolute configurations: (a) (*S*)-2-butanol; (b) (*R*)-2-methyl-3-heptanol.

In the case of 2-butanol shown in Figure 17 (a), the chiral carbon atom has four substituents, i.e., #1 hydroxyl, #2 ethyl, #3 methyl, and #4 proton, which are ordered as shown, according to the sequence rule, i.e., atomic number of directly attached atoms in the periodic table. The ethyl group has a higher position than the methyl group.

In the projection of the molecule, the fourth substituent, a proton here, is placed at the rear side, and the molecule is viewed from the front side as shown in Figure 17 (a). The three substituents, #1 hydroxyl, #2 ethyl, #3 methyl, are arranged in a counter-clockwise manner, and hence its absolute configuration is defined as (*S*).

It should be noted that the sequence rule is a little complex, as exemplified in the case of (*R*)-2-methyl-3-heptanol, where *iso*-propyl and *n*-butyl groups are compared (Figure 17 (b)). In the first sphere directly attached to the chiral carbon, both groups have a carbon

atom, respectively. In the second sphere, the *iso*-propyl group has two carbon atoms and one hydrogen atom, while the *n*-butyl group has one carbon atom and two hydrogen atoms. Therefore, the *iso*-propyl group has a priority, and hence the three groups make a clockwise rotation as shown. So, the absolute configuration of the present compound is defined as (*R*).

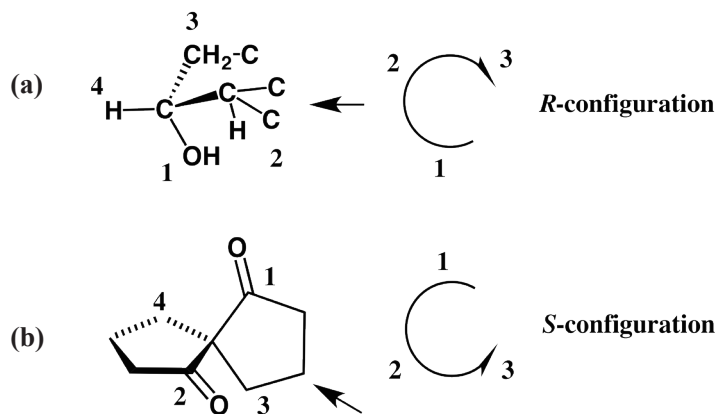
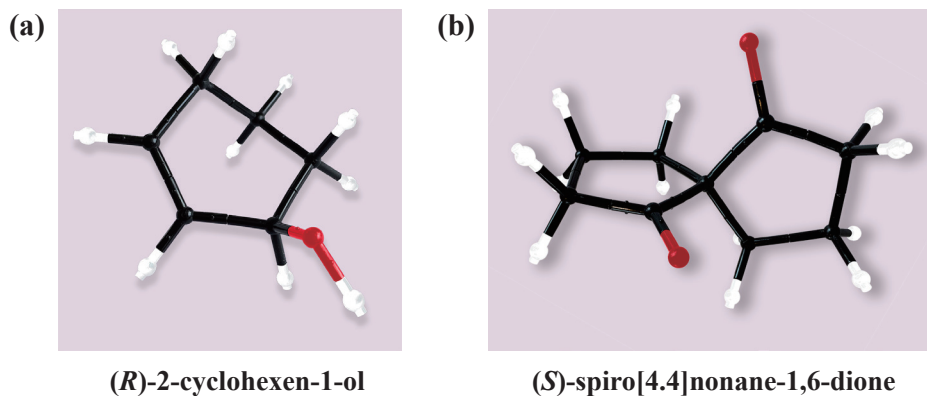


Figure 18

The models of chiral compounds and the definition of (*R*)- and (*S*)-absolute configurations: (a) (*R*)-2-cyclohexen-1-ol; (b) (*S*)-spiro[4.4]nonane-1,6-dione.

When a C=C double bond is contained in a chiral compound, the definition of (*R*)- or (*S*)-absolute configuration is performed as exemplified in Figure 18 (a). In the case of 2-cyclohexen-1-ol, the sequence rule defines that the olefinic carbon atom at the position 2 has two carbon atoms and one hydrogen atom. Namely, it is defined that in the C=C double bond, the π -bond also has an additional carbon atom, in addition to the σ -bond. Therefore, the absolute configuration of the present 2-cyclohexen-1-ol is defined as (*R*).

Spiro compounds with central chirality are very interesting as exemplified in Figure 18 (b), where spiro[4.4]nonane-1,6-dione is depicted. The central chiral carbon has two carbonyl moieties and two methylene moieties, where carbonyl group is higher than methylene group. So, if one carbonyl group is selected as #1, the remaining carbonyl group is defined as #2.

Between two methylene groups, the one group contained in the same ring with #1 carbonyl group has a priority, i.e., #3. The remaining methylene group is assigned as #4. Therefore, the absolute configuration of the present spiro[4.4]nonane-1,6-dione is defined as (*S*).

In the above definition, the carbonyl group in the right ring was selected as #1. However, even if the carbonyl group of the left ring is selected as #1, the conclusion is the same, because of the C_2 -symmetrical nature of this spiro compound.

In a similar manner, the (*1R,4R*)-absolute configuration of (+)-camphor shown in Figure 14 is easily recognized by using its molecular model.

In Conclusion

As explained above, HGS stereochemistry molecular models are very useful for students and researchers to study molecular structures, especially three-dimensional structures, i.e., stereochemistry, including absolute configurations. Since the models contain bonds already united with atoms, the stereochemistry models are handy for constructing various molecules. Therefore, HGS stereochemistry molecular model sets are one of the best available molecular models and indispensable for stereochemical studies by students and researchers. Please visit our website.

<https://hgs.maruzen.info/>
Email: hgshelp@maruzen.info



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Important Notice:

With a new manufacturer and improved production process, our stereochemistry molecular model set #4010 has upgraded to the new “ α (Alpha)” series. Please be advised that the new set is NOT compatible with any previous sets or parts.

Safety Guidelines:

1. Do not put the parts into orifices such as mouths, nostrils, ears, etc.
2. Keep the parts away from small children.
3. Do not give the parts to small children as misuse could result in permanent injury to the child.
4. Do not use the parts near fire, flame, or hot surfaces.
5. Recycle the plastic rather than dispose of it in the garbage.
6. Protect our environment; do not throw the product or its parts into a river, sea, or any body of water.

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110B Meadowlands Parkway, Suite 205
Secaucus, NJ 07094, USA