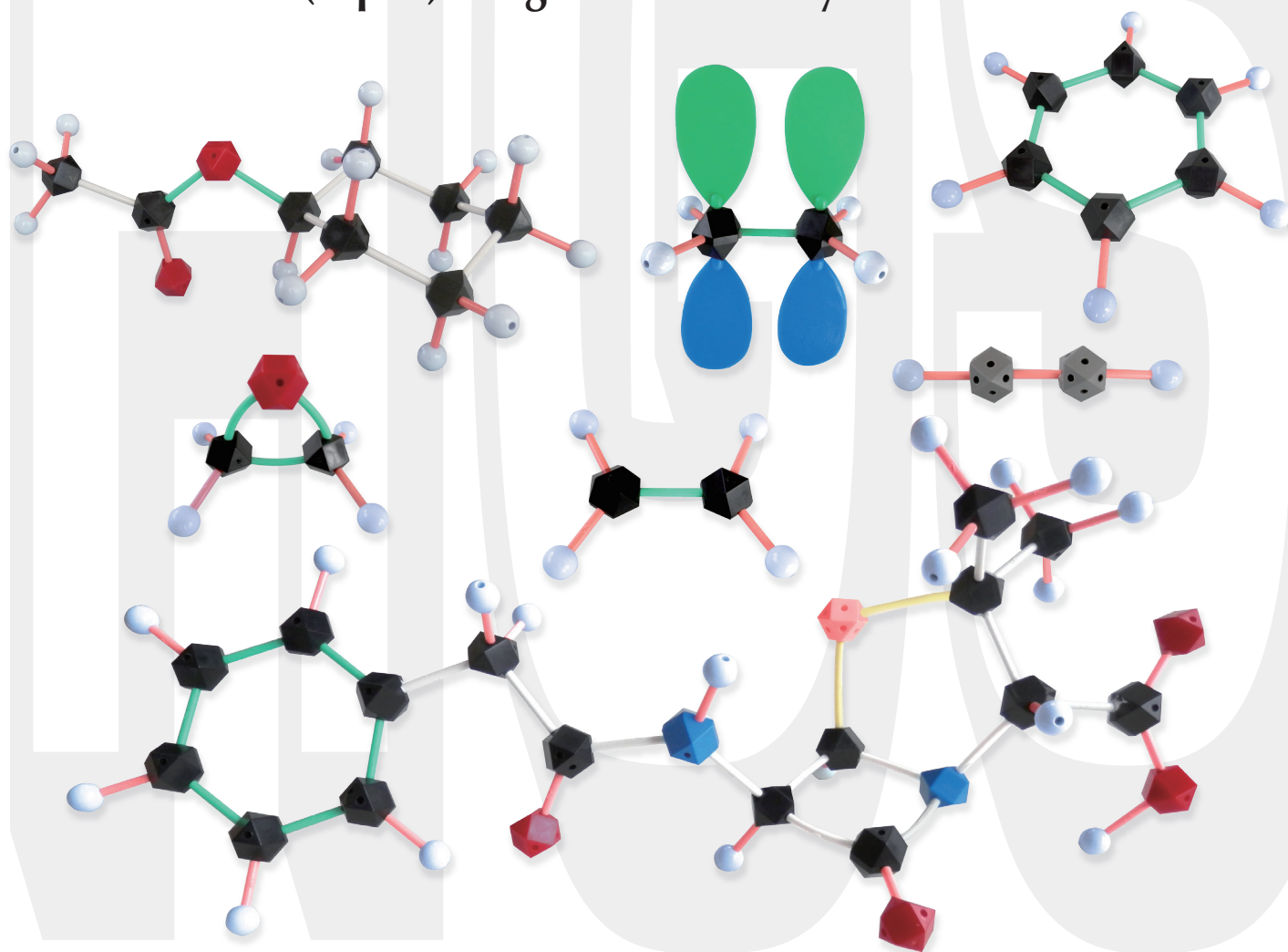


HGS

# POLYHEDRON MOLECULAR MODEL

## *New Alpha Series Manual 3<sup>rd</sup> Edition*

- #1000 $\alpha$ (Alpha) Fundamental Organic Chemistry Set
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**MARUZEN**

Tokyo, Japan

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# Polyhedron Molecular Model Sets: Contents

## Atom

Item No.	Atom Name	Color	Use	Quantity					
				#1000 $\alpha$	#1001 $\alpha$	#1002 $\alpha$	#1013 $\alpha$ 3rd Edition	#1003 $\alpha$ 2nd Edition	#1005 $\alpha$ 3rd Edition
ATM-01	H	white	s	30	24	24	30	30	72
ATM-11	B	orange	$sp^2, dsp^3$	-	-	-	-	-	1
ATM-02	C( $sp^3$ )	black	$sp^3$	12	12	12	12	28	46
ATM-09	C( $sp^2$ )	black	$sp^2, dsp^3$	-	3	-	6	12	20
ATM-03	N( $sp^3$ )	blue	$sp^3$	2	6	2	1	3	5
ATM-10	N( $sp^2$ )	blue	$sp^2, dsp^3$	-	-	-	1	3	5
ATM-04	O	red	$sp^3$	6	2	2	4	7	12
ATM-05	Si	yellow green	$sp^3$	-	-	-	-	-	1
ATM-06	P	yellow	$sp^3$	-	-	-	-	1	2
ATM-07	S	pink	$sp^3$	-	-	-	1	1	2
ATM-08	Cl	green	$sp^3$	2	2	-	1	2	4
ATM-17	m( $sp$ )	gray	$sp, sp^3, d^2sp^3$	-	3	1	2	2	4

## Bond (1 Å = 2.5 cm)

Item No.	Bond Length (Å)	Color	Use	Quantity					
				#1000 $\alpha$	#1001 $\alpha$	#1002 $\alpha$	#1013 $\alpha$ 3rd Edition	#1003 $\alpha$ 2nd Edition	#1005 $\alpha$ 3rd Edition
BND-02	1.09*1	pink	C-H	30	25	25	30	30	72
	1.21*2		C $\equiv$ C, C=O						
BND-04	1.40	green	C=C, C-O C(ar)=C(ar)	-	-	-	8	16	38
BND-06	1.54	white	C-C, S-O	20	20	20	24	40	72
BND-07	1.80	yellow	C-P C-Cl, C-S	-	-	-	2	8	20
BND-09	2.10	white	C-I	-	-	-	-	-	2
BND-10 (bent bond)	1.33	blue	C=C	12	6	6	10	12	30

\*1) In the case of C-(#2 bond)-H, bond length = 1.09 Å.

\*2) In the case of C-(#2 bond)-(non-H atom), bond length = 1.21 Å.

## Orbital Plate

Item No.	Color	Use	Quantity					
			#1000 $\alpha$	#1001 $\alpha$	#1002 $\alpha$	#1013 $\alpha$ 3 <sup>rd</sup> Edition	#1003 $\alpha$ 2 <sup>nd</sup> Edition	#1005 $\alpha$ 3 <sup>rd</sup> Edition
OBP-1	blue	p-atomic orbital	-	-	-	2	4	6
OBP-2	green	p-atomic orbital	-	-	-	2	4	6
OBC-1	blue	orbital connector	-	-	-	-	-	3
OBC-2	green	orbital connector	-	-	-	-	-	3

## Tool

Item	Quantity					
	#1000 $\alpha$	#1001 $\alpha$	#1002 $\alpha$	#1013 $\alpha$ 3 <sup>rd</sup> Edition	#1003 $\alpha$ 2 <sup>nd</sup> Edition	#1005 $\alpha$ 3 <sup>rd</sup> Edition
Bond puller (black)	1	1	1	1	1	1
Ruler (1 Å = 100 pm = 2.5 cm)	-	-	-	-	1	1


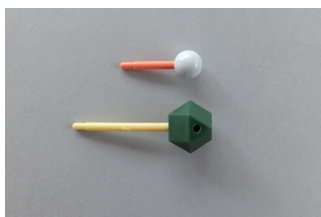

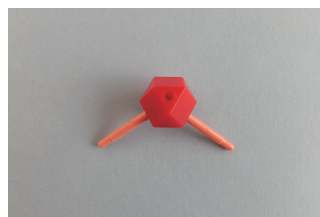

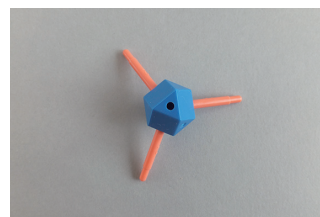
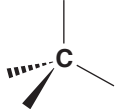
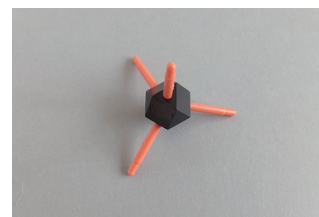
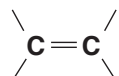
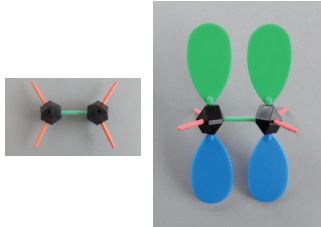

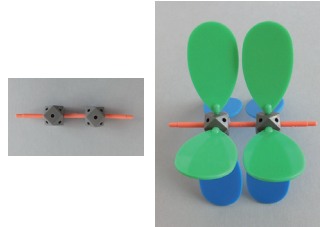

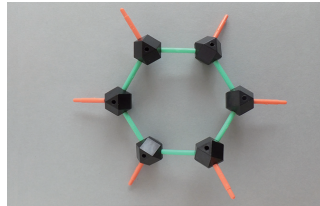
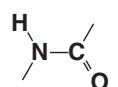
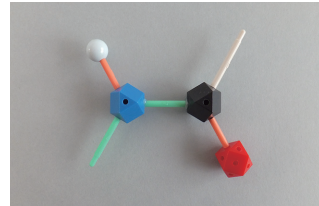

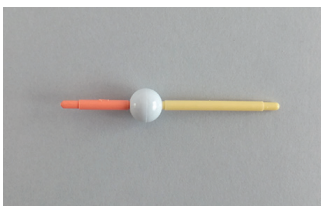
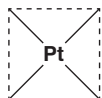
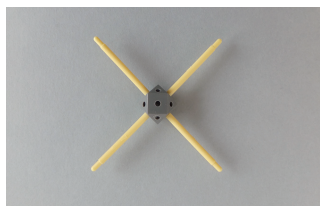
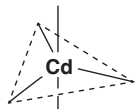
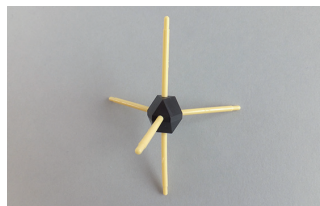
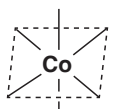
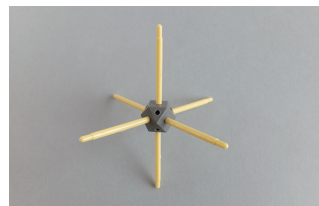
**Note:** This manual was prepared for the HGS polyhedron molecular models as a general guidance. Therefore, all the kits **1000 $\alpha$** , **1001 $\alpha$** , **1002 $\alpha$** , **1013 $\alpha$** , **1003 $\alpha$** , and **1005 $\alpha$**  do not necessarily contain the parts used for constructing the molecular models shown in this manual. For details, see the above tables. The latest versions of the tables can be found on our online shop (<http://hgs.maruzen.info/>).



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

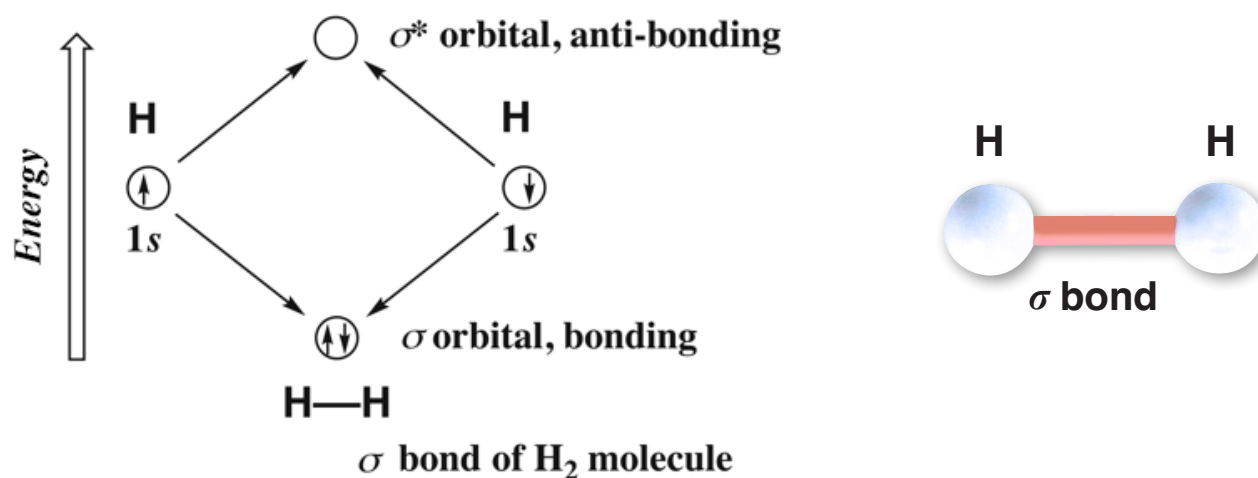
$(sp^3)$ C – C ( $sp^3$ )	1.54	C = O (ester)	1.20
$(sp^3)$ C – C ( $sp^2$ )	1.51	$(sp^3)$ C – N ( $sp^3$ )	1.47
$(sp^3)$ C – C ( $sp$ )	1.46	$(sp^2)$ C = N	1.28
$(sp^2)$ C – C ( $sp^2$ )	1.46	$(sp)$ C $\equiv$ N	1.14
(ar) C $\equiv$ C (ar)	1.39	$(sp^3)$ C – S ( $sp^3$ )	1.82
$(sp^2)$ C = C ( $sp^2$ )	1.34	$(sp^2)$ C = S	1.67
$(sp)$ C $\equiv$ C ( $sp$ )	1.18	$(sp^3)$ C – P ( $sp^3$ )	1.86
$(sp^3)$ C – H	1.09	$(sp^3)$ C – Si ( $sp^3$ )	1.86
$(sp^2)$ C – H	1.08	$(sp^3)$ C – F	1.40
$(sp^3)$ C – OH	1.43	$(sp^3)$ C – Cl	1.80
RC(=O) – OR	1.34	$(sp^3)$ C – Br	1.97
RC(=O) – OH	1.31	$(sp^3)$ C – I	2.14
RC(=O)O – R	1.44	O – H (alcohol)	0.97
R – OR	1.43	O – H (acid)	1.02
(ar) C – OR	1.36	N – H (amine)	1.01
C = O (ketone)	1.21	N = O (nitro)	1.22

# Hybrid Orbital and Molecular Structure

<p>atom with one bond</p> <p>H, Cl<sup>4</sup>, etc. </p> 	<p><math>sp^3</math> atom with two bonds</p> <p>O<sup>4</sup>, S<sup>4</sup>, etc. </p> 	<p><math>sp^3</math> atom with three bonds</p> <p>N<sup>4</sup>, P<sup>4</sup>, etc. </p> 	<p><math>sp^3</math> atom with four bonds</p> <p>C<sup>4</sup>, Si<sup>4</sup>, etc. </p> 
<p>double bond with <math>sp^2</math> atoms</p> <p>C<sup>5</sup><sub>20</sub>, etc. </p> 	<p>triple bond with <math>sp</math> atoms</p> <p>m<sup>14</sup>, etc. </p> 	<p>benzene ring with <math>sp^2</math> atoms</p> <p>C<sup>5</sup><sub>20</sub>, etc. </p> 	<p>amide group with <math>sp^2</math> atoms</p> <p>N<sup>5</sup><sub>20</sub>, C<sup>5</sup><sub>20</sub>, etc. </p> 
<p>hydrogen bond</p> <p>H </p> 	<p><math>dsp^2</math> metal complex, square planar</p> <p>m<sup>14</sup> </p> 	<p><math>dsp^3</math> metal complex, trigonal bipyramidal</p> <p>C<sup>5</sup><sub>20</sub> </p> 	<p><math>d^2sp^3</math> metal complex, octahedral</p> <p>m<sup>14</sup> </p> 

# 1. Molecular Structure: Covalent Bond Formation

The 20th century brought many progresses in science and technology, and the development of Quantum Mechanics in physics and chemistry is especially important. In chemistry, the structures of molecules were explicitly clarified by introducing the concept of a covalent bond based on the quantum mechanics. For example, the mechanism by which two neutral hydrogen atoms can combine with each other to make a molecule of  $H_2$  had been a problem of classical mechanics for a long time. But it was solved by quantum mechanics; namely two hydrogen nuclei share two electrons to make a covalent bond between two neutral atoms (**Figure 1**).



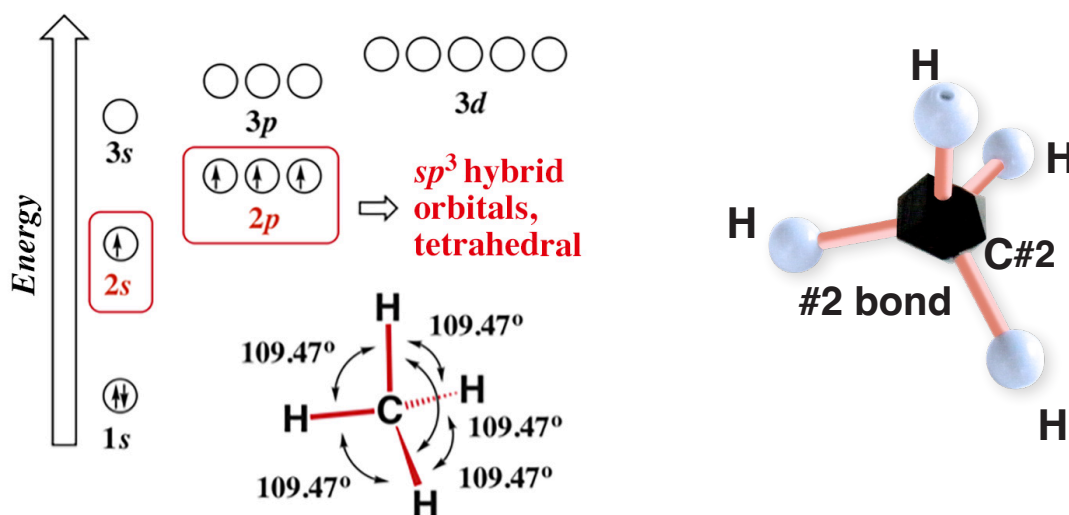
**Figure 1**  
The  $\sigma$  bond formation of  $H_2$  molecule

The  $1s$  electron of a hydrogen H atom interacts with that of the other H atom to form a  $\sigma$  bond between two H nuclei as shown in **Figure 1**, where the  $\sigma$  orbital with bonding character is formed from two atomic  $1s$  orbitals. The  $\sigma$  orbital is filled with two electrons to make a  $\sigma$  bond, and the bonding energy is released to stabilize the  $H_2$  molecule. This is the formation mechanism of a covalent bond between two H atoms.

The model of  $H_2$  molecule is shown in **Figure 1**, where two balls (H#1) representing H nuclei are connected by a stick (#2 bond) representing the  $\sigma$  bond. Although the experimental bond length is  $0.741 \text{ \AA}$ , the bond is approximated by #2 bond (H-H bond length  $0.98 \text{ \AA}$ ) here. It should be noted that the scale of the Polyhedron Model is  $1 \text{ \AA} = 2.5 \text{ cm}$ .

## 2. Molecular Structure: Atomic Orbital Hybridization, Bond Angle, and Bond Length

The molecular structure of methane CH<sub>4</sub>, a simple organic compound, was similarly explained based on the quantum mechanics as follows. The atomic orbitals of a C atom are shown in **Figure 2**, where each of one 2s and three 2p atomic orbitals has an unpaired electron indicating the tetravalent C atom. One 2s and three 2p atomic orbitals make four  $sp^3$  hybrid orbitals, which take the tetrahedral configuration as exemplified by the case of methane molecule.



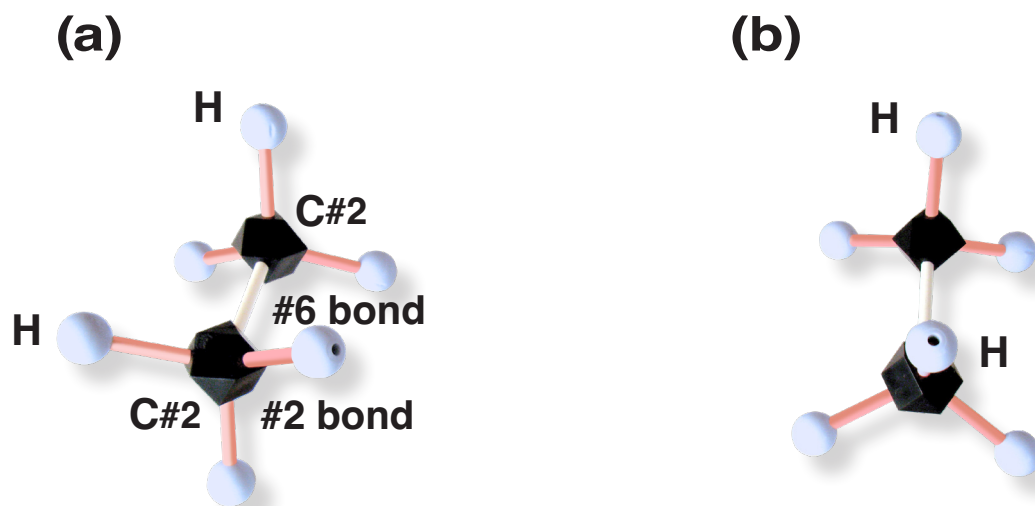
**Figure 2**  
The atomic orbitals and energy levels of an alkane carbon atom, from which four new  $sp^3$  hybrid orbitals (red color) are formed taking a tetrahedral structure as exemplified by a methane molecule, where all bond angles H-C-H are 109.47°

In methane molecule, the central C atom makes covalent bonds with four hydrogen atoms to produce a tetrahedral structure. This bonding is called the tetrahedral  $sp^3$  orbital hybridization, where the hydrogen-carbon-hydrogen bond angle is 109.47°. To construct the methane molecular model, four H#1 atom parts are connected to a tetrahedral  $sp^3$  carbon atom, C#2, with #2 bonds (bond length 1.09 Å) as shown in **Figure 2**. Although the experimental bond length (exp. BL) between C and H atoms is 1.06 Å, it is thus approximated by the #2 bond.

### 3. Alkanes, Saturated Hydrocarbons and Conformational Change

Ethane molecule is made of two  $sp^3$  carbon atoms and six hydrogen atoms as shown in **Figure 3**, where two  $sp^3$  carbon atoms (C#2) are connected to each other by a white #6 bond (1.54 Å). Six hydrogen atoms (H#1) are connected to  $sp^3$  carbon atoms by pink #2 bonds. Unlike methane, ethane has conformational mobility. Namely, ethane molecule takes the most stable staggered conformation (the dihedral angle H-C-C-H is  $60^\circ$  as shown in **Figure 3**) and the less stable eclipsed conformation (the dihedral angle H-C-C-H is  $0^\circ$  as shown in **Figure 3**).

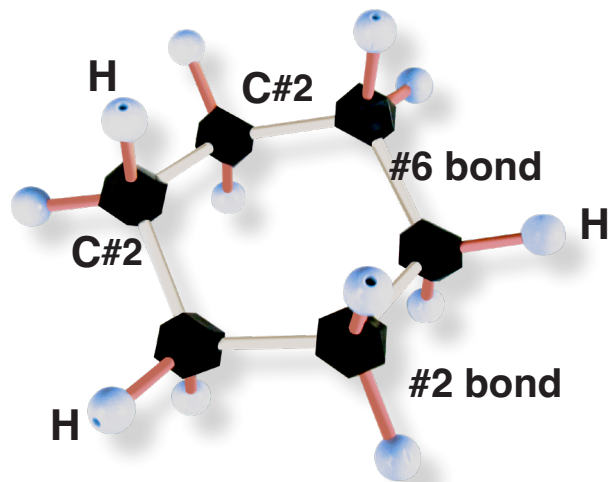
Because of the exact mechanical matching of hole and stick, the HGS polyhedron atoms can smoothly rotate around a bond stick connecting atoms, but the rotation needs a small force. Namely atoms do not freely rotate around a bond. Accordingly, the high quality HGS models are the best for demonstrating conformational changes. Therefore, it is easy to maintain specific conformations of flexible acyclic compounds, as exemplified by the models of staggered and eclipsed conformations of an ethane molecule (**Figure 3**).



**Figure 3**  
Molecular model of ethane:  
(a) staggered conformation  
(b) eclipsed conformation

The cyclohexane molecular model is similarly assembled with six  $sp^3$  tetrahedral carbon atoms (#2), which are connected by #6 bonds (**Figure 4**).



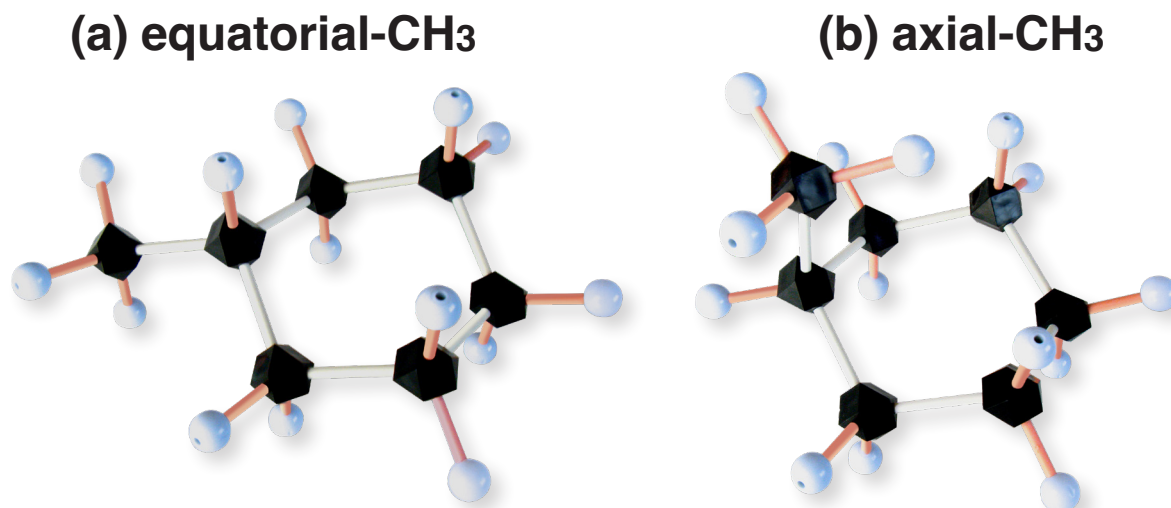


**Figure 4**  
Molecular model of cyclohexane (chair form)

Twelve hydrogen atoms (#1) are bonded to  $sp^3$  carbon atoms by #2 bonds. As is well known, cyclohexane takes the most stable chair form as shown in **Figure 4**.

The cyclohexane ring can undergo a conformational change between chair forms via a boat form. This cyclohexane ring “flip” can be easily performed using the HGS molecular model even by beginners. Namely, the ideal chair form and flipped chair form are readily obtained together with the boat form as an intermediate. This is one of the advantages of the HGS model.

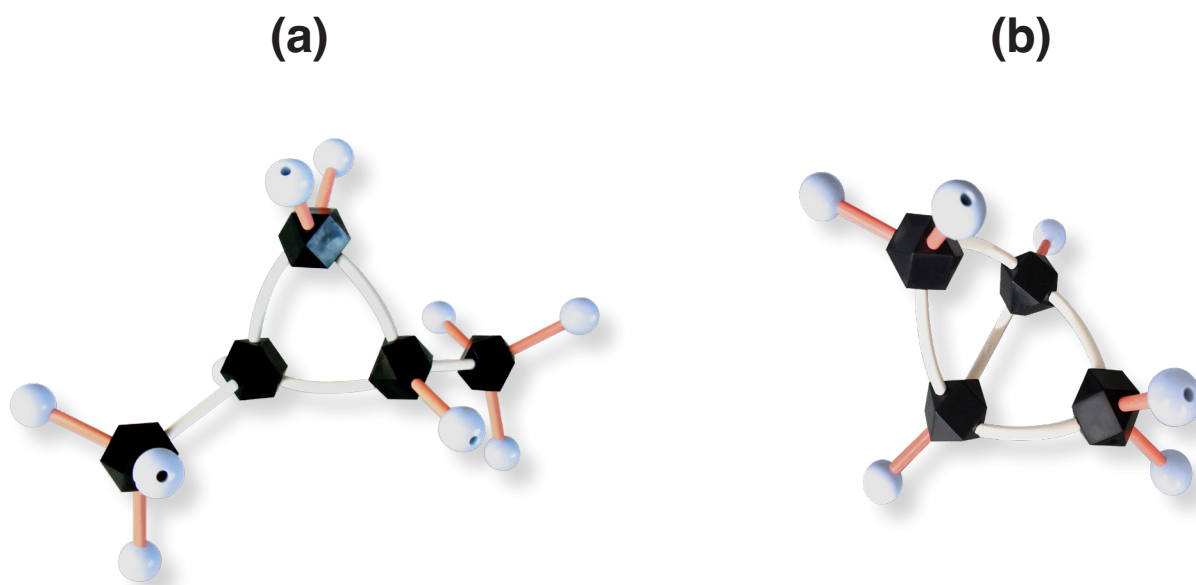
**Figure 5** shows two conformations of methylcyclohexane, where the equatorial-methylcyclohexane in (a) is more stable than the axial-methylcyclohexane in (b).



**Figure 5**  
Conformers of methylcyclohexane:  
(a) equatorial methylcyclohexane  
(b) axial methylcyclohexane

**Figure 6** (a) shows *trans*-1,2-dimethylcyclopropane, where #6 bonds (1.54 Å) are used for three-membered ring: experimental C-C bond length, 1.51 Å. It should be noted that according to the quantum mechanics, the bonds of a cyclopropane ring are out of the straight, taking the so-called bent bonds. The polyhedron model shown in **Figure 6** (a) mimics well the bent bonds.

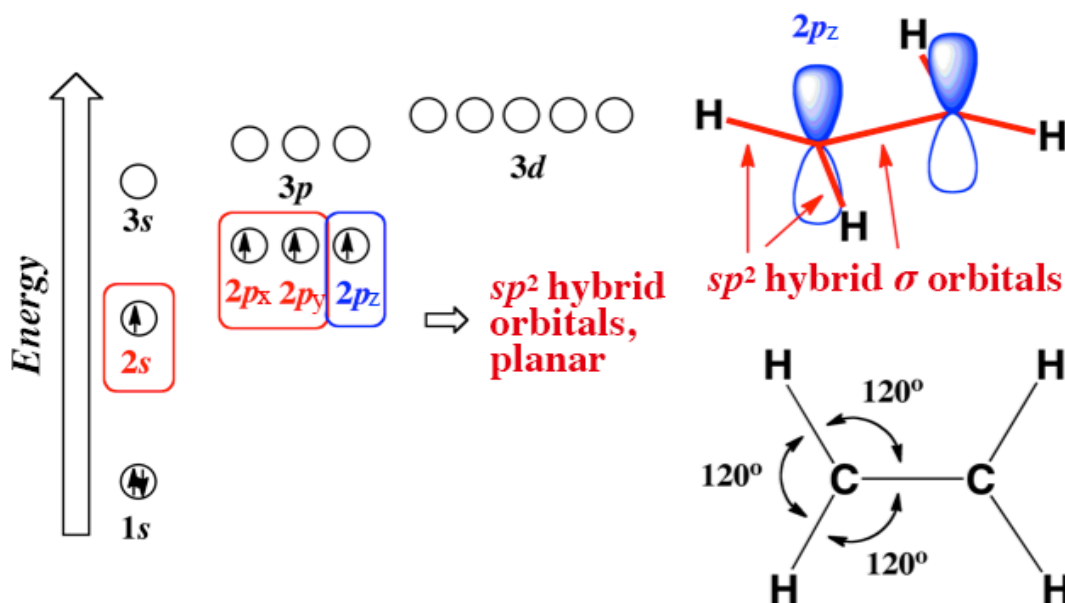
It is known that bicyclobutane, or bicyclo[1.1.0]butane, is one of the most strained compounds, because it is composed of two fused cyclopropane rings as shown in **Figure 6** (b). The HGS polyhedron model is thus very useful for constructing such a strained molecule, although the construction is not easy. It is advisable to make first a 3-membered ring and then to make another 3-membered ring; it is difficult to bond the C-atoms at positions 1 and 3 in a cyclobutane ring. If necessary, use a hair dryer to soften the plastic bonds.



**Figure 6**  
(a) *Trans*-1,2-dimethylcyclopropane  
(b) bicyclobutane

## 4. Alkenes and Aromatic Compounds

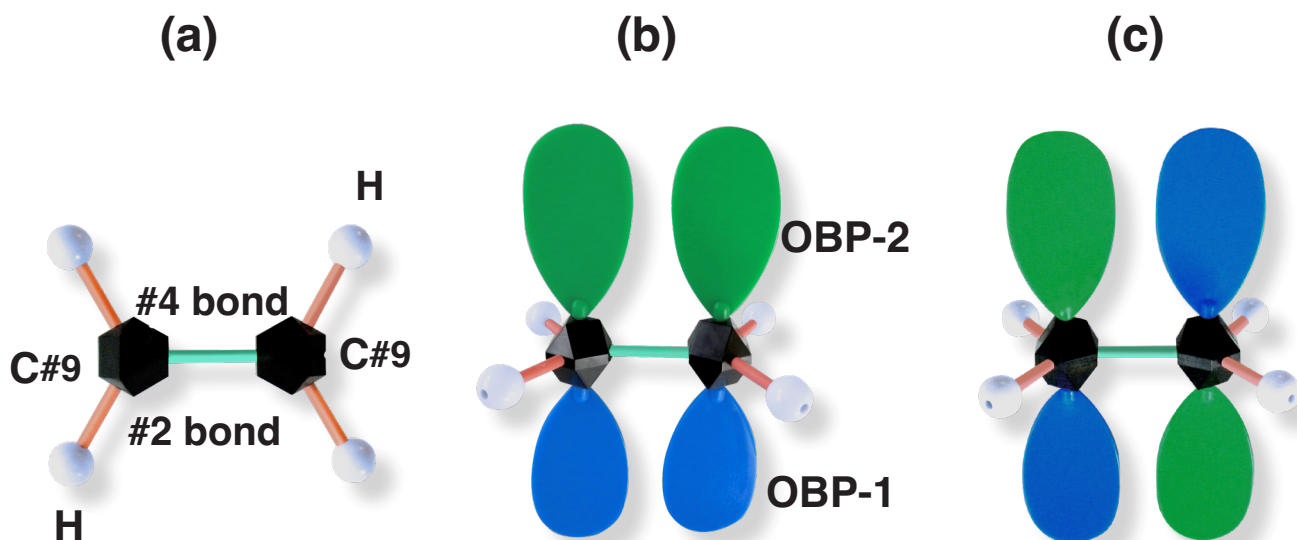
In the case of alkanes discussed above, a C atom takes tetrahedral  $sp^3$  orbitals. On the other hand, a C atom can take another configuration of  $sp^2$  hybrid orbitals, which are made of  $2s$ ,  $2p_x$  and  $2p_y$  atomic orbitals. It should be noted that the  $sp^2$  hybrid orbitals are placed in a plane and the angles between them are  $120^\circ$ . The remaining  $2p_z$  atomic orbital is used for making a  $\pi$ -bond (**Figure 7**).



**Figure 7**

The atomic orbitals and energy levels of an alkene carbon atom, where three new  $sp^2$  hybrid orbitals (red color) are formed and used as  $\sigma$  bonds taking a planar structure. The remaining  $2p_z$  orbital is perpendicular to the plane and used as a  $\pi$ -bond as exemplified by an ethylene molecule.

A typical example of  $sp^2$  hybridization and  $\pi$ -bond is seen in an ethylene molecule as shown below. The ethylene molecule is made of two  $sp^2$  carbon atoms and four hydrogen atoms as shown in **Figure 8** (a), where two  $sp^2$  C atoms (#9) are connected to each other by a #4 bond (1.40 Å,  $\sigma$  bond). As shown in **Table 1**, the experimental bond length of a C=C double bond is 1.34 Å and therefore, the #4 bond of 1.40 Å is used to a first approximation. Four hydrogen atoms (#1) are connected to  $sp^2$  carbon atoms by #2 bonds. All atoms of an ethylene molecule are thus located in a plane (**Figure 8**). The bond angles C-C-H and H-C-H are  $120^\circ$ .

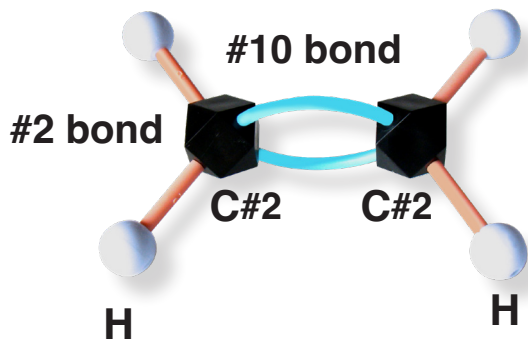


### Figure 8

Molecular model of ethylene: (a) showing the  $\sigma$  skeleton; (b) showing a  $\pi$ -MO of the ground state, where the same color indicates a bonding interaction; (c) showing a  $\pi$ -MO of the excited state, where different colors indicate an anti-bonding interaction

The molecular model of ethylene in **Figure 8** (a) shows only the  $\sigma$  skeleton. But in the HGS model, the  $\pi$ -bond, which governs the reactivity of olefin, can be made by using  $p$ -AO (atomic orbital) plates as shown in **Figure 8** (b). The  $p$ -AO plates (OBP-1, blue and OBP-2, green) are placed perpendicular to the  $\sigma$  skeleton plane of an ethylene molecule, satisfying the theoretical requirements. If the green and blue plates indicate the plus and minus signs of  $p$ -AOs, respectively, the  $\pi$ -MO (molecular orbital) formed by  $p$ -AOs shown in **Figure 8** (b) corresponds to the ground state, as expected from quantum mechanics.

On the other hand, the  $\pi$ -MO illustrated in **Figure 8** (c) shows the anti-bonding MO of the excited state, because the green (+)  $p$ -AO plate is next to the blue (-)  $p$ -AO plate. The HGS molecular model is thus useful for showing the correct structure and the bonding mechanism of a C=C double bond (**Figure 8**). After understanding the basic nature of double bond,  $p$ -AO plates become unnecessary for assembling larger molecules.

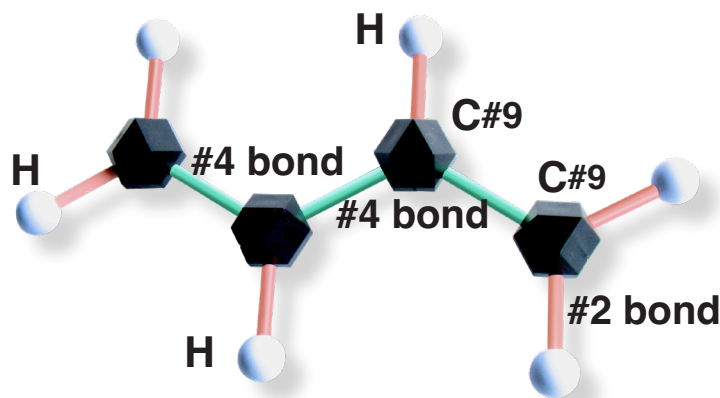


**Figure 9**  
Conventional molecular model  
of ethylene

In the model kits #1000 $\alpha$ , #1001 $\alpha$ , and #1002 $\alpha$ , the old C=C double bond is used, where two  $sp^3$  carbon atoms (#2) are connected by two bent bonds (#10, 1.33 Å) as shown in **Figure 9**. This double bond with two bent bonds has traditionally been used, because it easily visualizes the double bond (two bonds). However, such a simple visualization may be confusing to users, because this structure is scientifically and geometrically incorrect. Namely, in this structure, the bond angle H-C-H is 109°28', which obviously disagrees with the bond angle (120°) of the  $sp^2$  hybridization. In addition, both the difference between  $\sigma$  bond and  $\pi$ -bond and the quantum mechanical results described above cannot be explained by this structure.

In conclusion, we strongly recommend the Polyhedron Model kits 1013 $\alpha$ , 1003 $\alpha$ , and 1005 $\alpha$  containing  $sp^2$  C atoms (C#9) and #4 bonds (1.40 Å), so that the C=C double bond can be correctly assembled and explained.

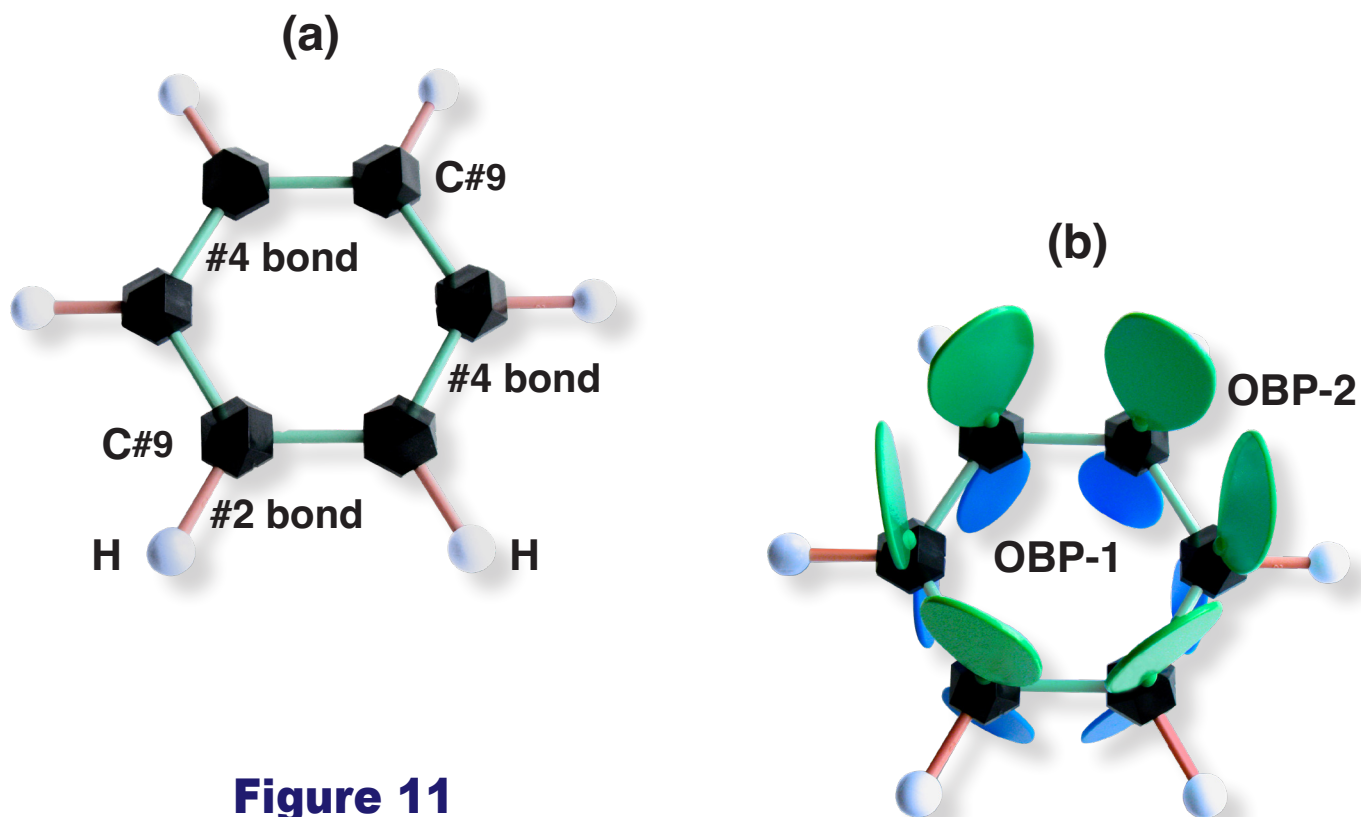
The molecule of 1,3-butadiene, a conjugated diene, is made of four  $sp^2$  carbon atoms and six hydrogen atoms as shown in **Figure 10**, where four  $sp^2$  C atoms (#9) are connected to one another by #4 bonds (1.40 Å). As the experimental bond lengths of the C=C double bond and C-C single bond in 1,3-butadiene are 1.33 Å and 1.46 Å, respectively, the #4 bonds of 1.40 Å are used to a first approximation. It should be noted that all atoms are placed in a single plane and the molecule takes the s-trans form.



**Figure 10**  
Molecular model of 1,3-butadiene with s-trans form

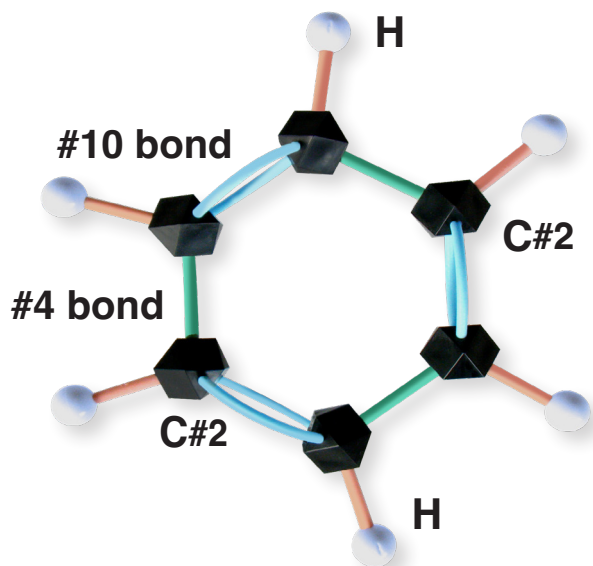
The benzene molecule is made of six  $sp^2$  carbon atoms (C#9) and six hydrogen atoms (#1) as shown in **Figure 11** (a), where all  $sp^2$  carbon atoms are connected to one another by #4 bonds (1.40 Å). The experimental bond length of a C=C aromatic bond in benzene is 1.39 Å and therefore, the #4 bonds are used to a first approximation. All carbon atoms make a regular hexagon and hence are placed in a single plane.

**Figure 11** (b) shows the  $\pi$ -MO of benzene, where six  $p$ -AO plates in the upper part are green and those in the lower part are blue. Therefore, the MO shown corresponds to the  $\pi$ -MO of the lowest energy.



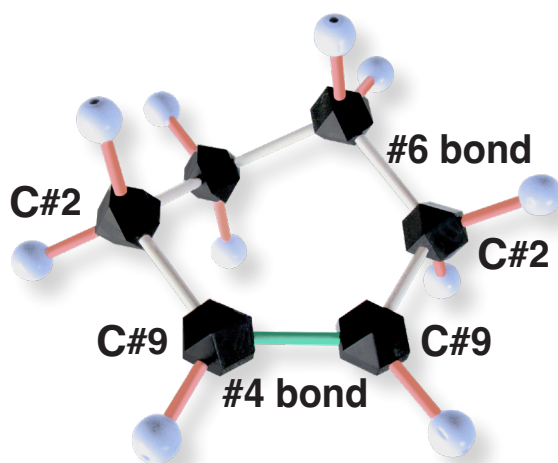
**Figure 11**  
**Molecular model of benzene:**  
**(a) showing the  $\sigma$  skeleton**  
**(b) showing the  $\pi$ -MO of the lowest energy level**

**Figure 12** shows the conventional model of benzene, where six  $sp^3$  carbon atoms (C#2) are connected by bent bonds (#10, 1.33 Å) and #4 bonds (1.40 Å) alternately. It is obvious that the benzene skeleton deviates from a regular hexagon, and especially the atoms H-C(1) ----- C(4)-H largely deviate from a straight line. Furthermore, it is impossible to explain the resonance or conjugation of  $\pi$ -electrons in the benzene ring by this model. These facts completely disagree with the physical and chemical characters of benzene, and hence these are the disadvantages of the conventional molecular model of benzene using tetrahedral C atoms and bent bonds.



**Figure 12**  
Conventional molecular model of benzene using bent bonds

We again strongly suggest using  $sp^2$  carbon atoms (C#9) and #4 bonds (1.40 Å) for constructing olefin and aromatic compounds. In this sense, HGS Polyhedron Model kits 1013 $\alpha$ , 1003 $\alpha$ , and 1005 $\alpha$  containing these parts are recommended.

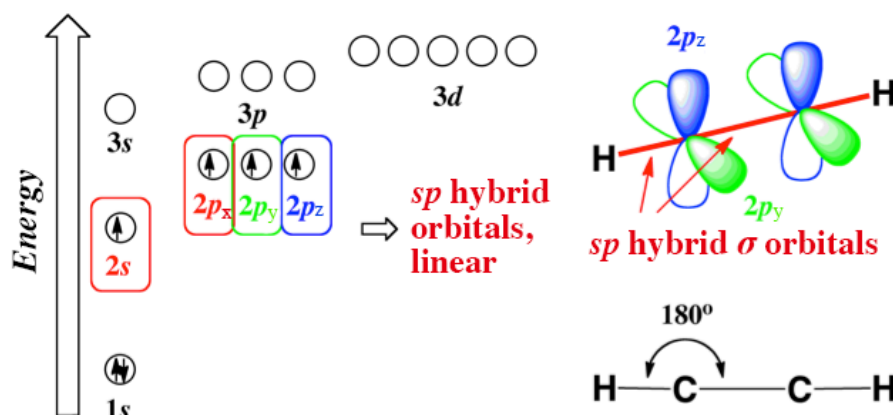


**Figure 13**  
Molecular structure of the half-chair form of cyclohexene

The stereo-structure of cyclohexene is illustrated in **Figure 13**, where the C-C=C-C moiety is planar. Therefore, the molecule takes a half-chair conformation as a stable conformer. When constructing alkene compounds, it is important to remember that the C-C=C-C moiety is planar.

## 5. Acetylene, an Alkyne Compound

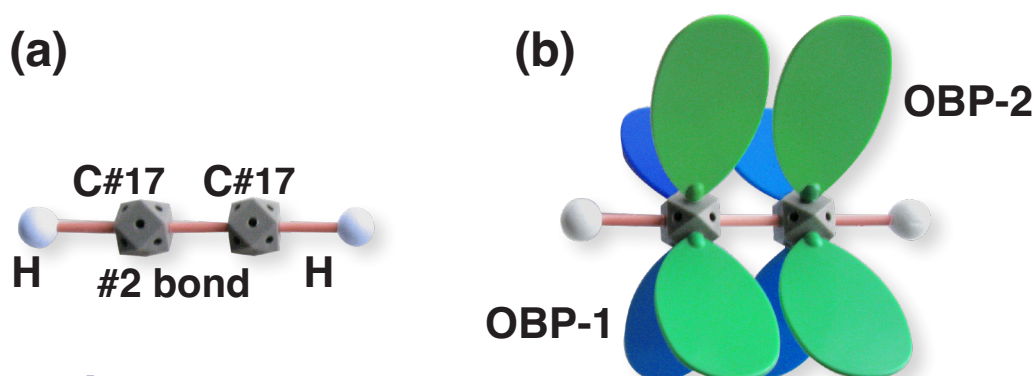
The third configuration of a C atom is seen in alkyne compounds, where 2s and  $2p_x$  atomic orbitals make  $sp$  hybrid orbitals as shown in **Figure 14**.



**Figure 14**

The atomic orbitals and energy levels of an alkyne carbon atom, where two new  $sp$  hybrid orbitals (red color) are formed and used as  $\sigma$  bonds taking a linear structure. The remaining  $2p_y$  and  $2p_z$  orbitals are perpendicular to the line and used as  $\pi$ -bonds as exemplified by an acetylene molecule.

It should be noted that the  $sp$  hybrid orbitals form a linear structure and the angles between them are  $180^\circ$ . The remaining  $2p_y$  and  $2p_z$  orbitals are used for making  $\pi$ -bonds (**Figure 14**).



**Figure 15**

Molecular model of acetylene:

(a) showing the  $\sigma$  skeleton

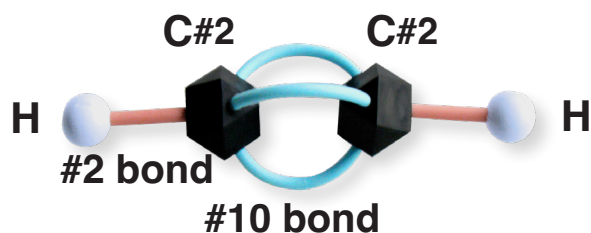
(b) showing two  $\pi$ -MOs, which are perpendicular to each other



An acetylene molecular model is made up of two  $sp$  carbon atoms and two hydrogen atoms as shown in **Figure 15** (a), where two  $sp$  carbon atoms (m#17) are connected to each other by a #2 bond (1.20 Å,  $\sigma$  bond).

As shown in **Table 1**, the typical bond length of  $C\equiv C$  triple bond is 1.18 Å and therefore, the #2 bond of 1.20 Å is used to a first approximation. Two hydrogen atoms (#1) are connected to  $sp$  carbon atoms by #2 bonds (1.09 Å): the typical bond length of ( $sp$ ) C-H bond is 1.08 Å. The acetylene molecule is thus linear (**Figure 15** (a)). The m#17 atom was originally designed as a metal atom of  $d^2sp^3$  hybridization, but it can also be used as a C atom of  $sp$  hybrid orbitals, which are made of the  $2s$  and  $2p$  atomic orbitals. The remaining two  $2p$  atomic orbitals are used as  $\pi$ -bonds. Thus, m#17 atom can be used as the  $sp$  C atom (C#17).

**Figure 15** (b) shows two  $\pi$ -MOs of an acetylene molecule, which are perpendicular to each other. The HGS model is thus useful for showing the correct structures of a molecule with  $\pi$ -MOs.



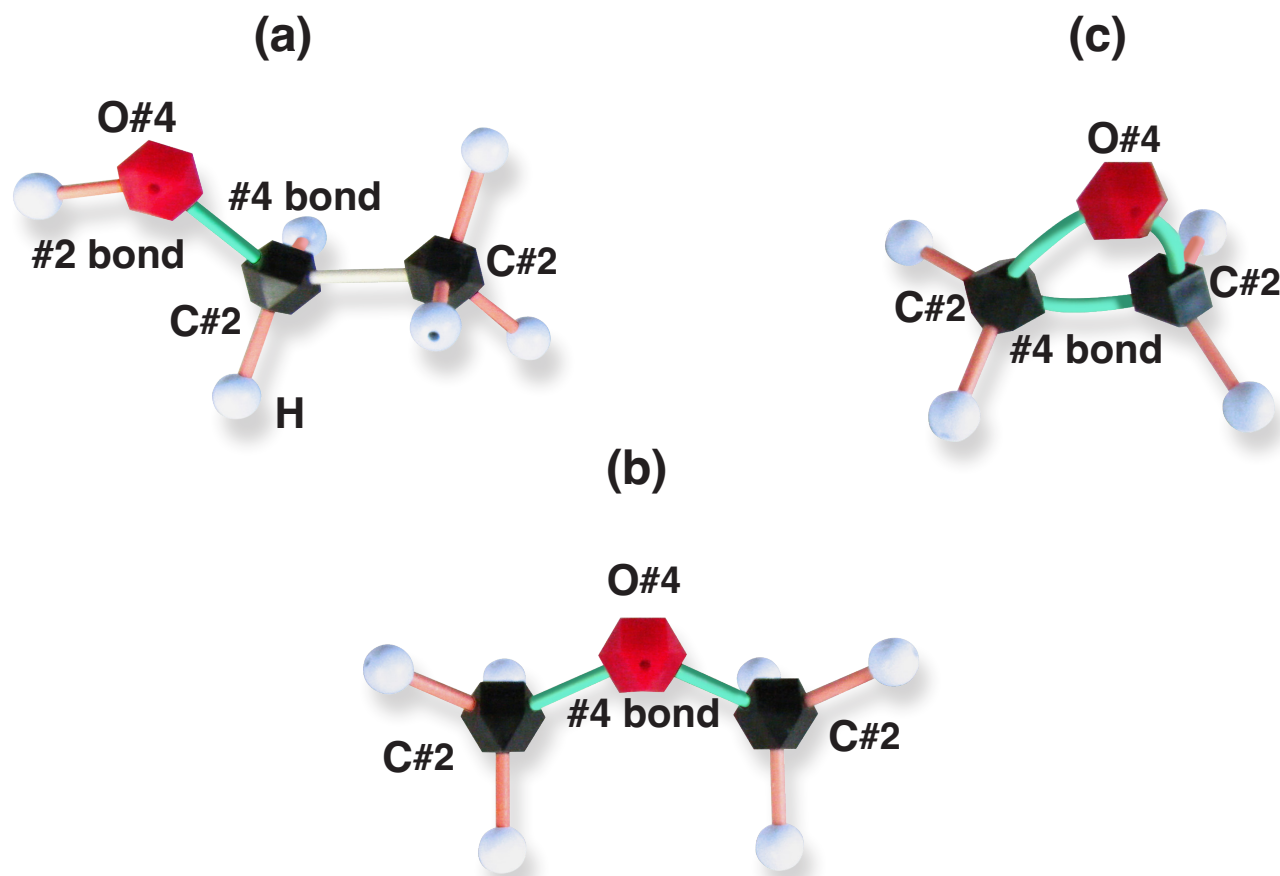
**Figure 16**  
Conventional molecular model of acetylene

The conventional model of an acetylene molecule is illustrated in **Figure 16**, where bent bonds are used for the triple bond. Again this triple bond model is scientifically incorrect.

## 6. Alcohols, Ethers, Ketones, and Esters

As an example of alcohols, the molecule of ethyl alcohol is shown in **Figure 17 (a)**, where two  $sp^3$  C atoms (C#2) are connected to each other by a #6 bond (1.54 Å), and a red  $sp^3$  oxygen atom (O#4) is connected to an  $sp^3$  carbon atom by a #4 bond (1.40 Å). The experimental bond length of the alcoholic C-O bond is 1.43 Å and therefore, the #4 bond is used to a first approximation. Since the experimental bond length of the alcoholic O-H bond is 0.97 Å, a #2 bond (1.09 Å) is used.

**Figure 17 (b)** illustrates the molecular structure of dimethyl ether, where a red  $sp^3$  oxygen atom (O#4) is connected to two  $sp^3$  carbon atoms (C#2) by #4 bonds (1.40 Å), because the experimental bond length of the ether C-O bond is 1.43 Å.

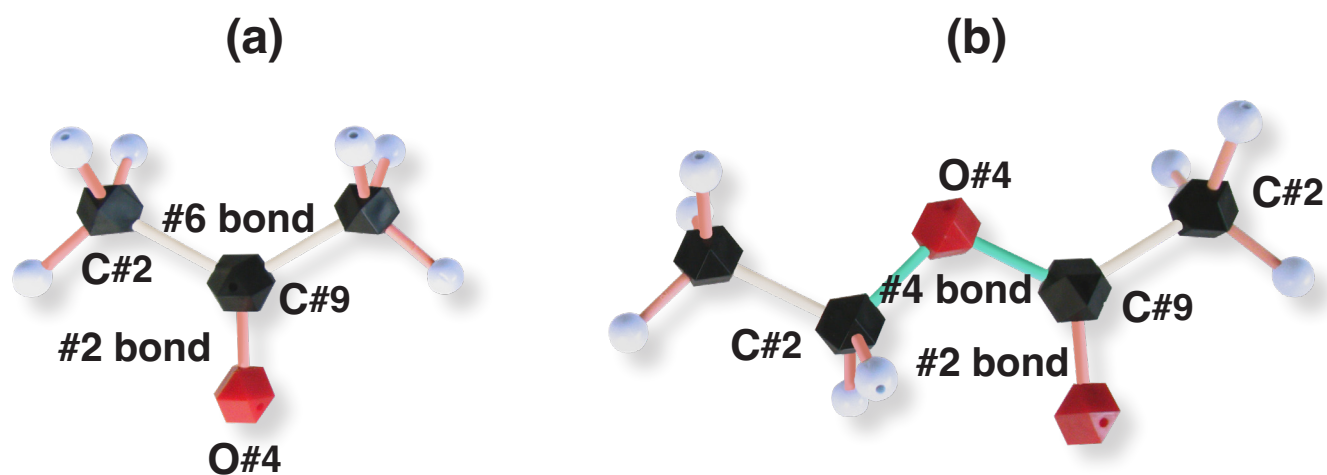


**Figure 17**  
Molecular models of ethyl alcohol,  
dimethyl ether, and ethylene oxide

**Figure 17 (c)** shows the molecular model of ethylene oxide, where a red  $sp^3$  oxygen atom (O#4) is connected to two  $sp^3$  carbon atoms (C#2) by #4 bonds (1.40 Å): the experimental bond length of the C-O bond is 1.43 Å. The  $sp^3$  carbon atoms (C#2) are connected to each other also by #4 bonds (1.40 Å): the experimental bond length of the C-C bond is 1.47 Å.

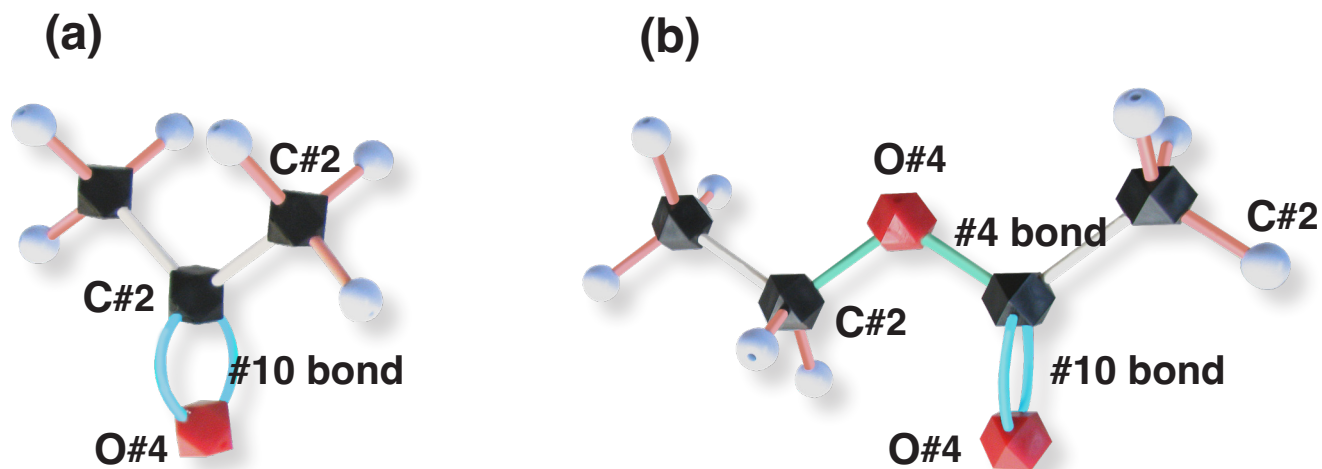
**Figure 18 (a)** depicts the molecular structure of acetone, where the  $sp^2$  carbon atom (C#9) of the carbonyl group is connected to two  $sp^3$  carbon atoms (C#2) of the methyl groups by #6 bonds (1.54 Å): experimental bond length, 1.49 Å. The  $sp^2$  carbon atom is connected to a red oxygen atom (O#4) by a #2 bond (1.21 Å) to represent the C=O double bond: experimental bond length, 1.21 Å.

In this model, the red  $sp^3$  oxygen atom was used for the C=O oxygen atom to a first approximation. This approximation is good only when the molecular geometry is considered. However, this is incorrect from the viewpoint of molecular orbital theory, which suggests that the  $sp^3$  oxygen atom has to be replaced by a #17 atom with  $sp$  hybridization.



**Figure 18**  
Molecular models of acetone and ethyl acetate

**Figure 18 (b)** shows the molecular structure of ethyl acetate, where the  $sp^3$  carbon atom (C#2) of the methyl group is connected to an  $sp^2$  carbon atom (C#9) by a #6 bond. The  $sp^2$  carbon atom is connected to an oxygen atom by a #2 bond (1.21 Å) to represent the ester C=O double bond: experimental bond length, 1.20 Å. The  $sp^2$  carbon atom is further connected to another oxygen atom by a #4 bond (1.40 Å) to represent the C–O single bond: experimental bond length, 1.34 Å. The second oxygen atom is further connected to the  $sp^3$  carbon atom of the ethyl group by a #4 bond (1.40 Å), because the experimental bond length of the ether C-O bond is 1.44 Å. It should be noted that the C–C(=O)–O–C moiety should be planar and take the stable conformation as shown in **Figure 18 (b)**.

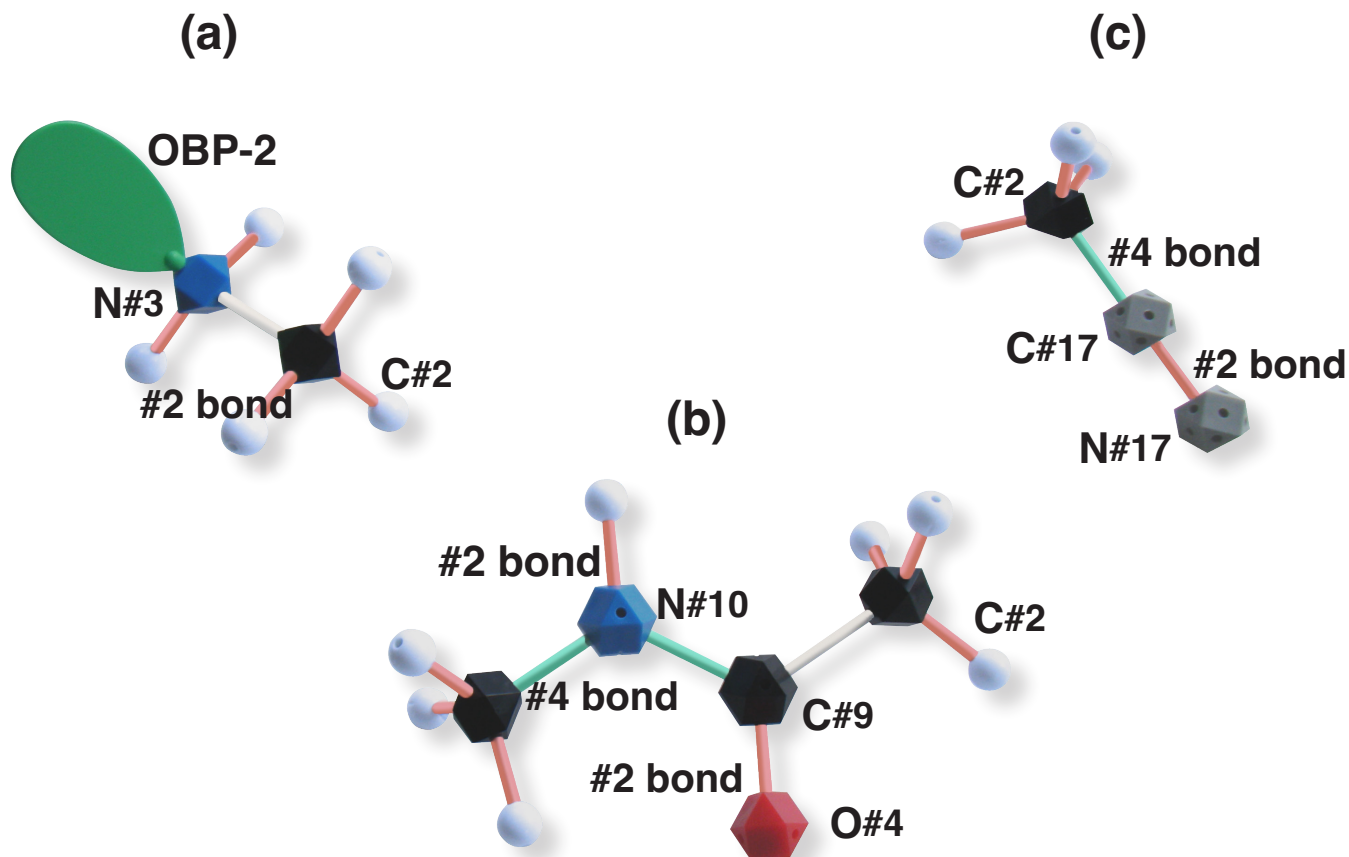


**Figure 19**  
 Conventional molecular models of acetone and ethyl acetate using bent bonds

**Figure 19** shows the conventional molecular models of acetone and ethyl acetate, where the C=O group is assembled by tetrahedral  $sp^3$  carbon and oxygen atoms together with bent bonds. However, as described above, the use of tetrahedral atoms and bent bonds for the double bond groups is incorrect from the viewpoint of geometry and the quantum mechanical theory. For example, the bond length of the C=O group assembled by bent bonds (#10) becomes 1.33 Å, which is longer than the experimental one (1.21 Å). Thus, the models using #2 bonds (1.21 Å) shown in **Figure 18** are much better than those in **Figure 19**. Therefore, we strongly suggest to use  $sp^2$  carbon atom (C#9) and #2 bond contained in the kits 1013 $\alpha$ , 1003 $\alpha$ , and 1005 $\alpha$ .

## 7. Amines, Amides, and Nitriles

As an example of amines, the molecule of methylamine is shown in **Figure 20** (a), where an  $sp^3$  carbon atom (C#2) is connected to a blue  $sp^3$  nitrogen atom (N#3) by a #6 bond (1.54 Å): experimental C-N bond length, 1.47 Å. The nitrogen atom is connected to two hydrogen atoms by #2 bonds (1.09 Å): experimental N-H bond length, 1.01 Å. The lone-pair electrons of the nitrogen atom attach at the remaining hole as shown in **Figure 20** (a), where a  $p$ -AO plate (OBP-2) represents the lone-pair electrons.



**Figure 20**  
**Molecular models of methylamine, *N*-methylacetamide,  
 and acetonitrile**

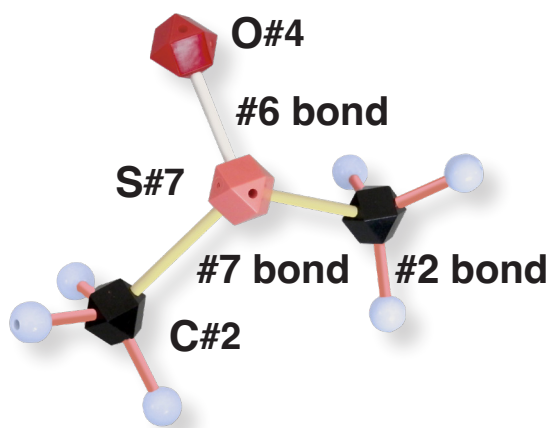
**Figure 20 (b)** illustrates the molecular model of *N*-methylacetamide, where the planar blue  $sp^2$  nitrogen atom (N#10) is connected to a black  $sp^2$  carbon atom (C#9) by a #4 bond (1.40 Å): experimental bond length, 1.33 Å. The  $sp^2$  carbon atom is connected to an oxygen atom (O#4) by a #2 bond (1.21 Å) to represent the amide C=O double bond: experimental bond length 1.23 Å. The  $sp^2$  carbon atom is further connected to the methyl group by a #6 bond: experimental bond length, 1.50 Å. The  $sp^2$  nitrogen atom is connected to an  $sp^3$  carbon atom by a #4 bond (1.40 Å): experimental bond length, 1.45 Å. The  $sp^2$  nitrogen atom is further connected to a hydrogen atom by a #2 bond (1.09 Å): experimental bond length, 1.01 Å. It should be noted that the skeleton of this molecule [C-C(=O)-NH-C] is planar as shown in **Figure 20 (b)**. In addition, the planar  $sp^2$  nitrogen atom (N#10) is indispensable for constructing an amide group, and hence we strongly recommend the Polyhedron Model kits, 1013 $\alpha$ , 1003 $\alpha$ , and 1005 $\alpha$ .

**Figure 20 (c)** shows the molecular model of acetonitrile, where the  $sp^3$  carbon atom (C#2) of the methyl group is connected to a #17 atom (C#17) of  $sp$  hybridization by a #4 bond (1.40 Å): experimental bond length, 1.46 Å. Namely, the #17 atom is used as the  $sp$  carbon atom. The  $sp$  carbon atom is connected to another #17 atom of  $sp$  hybridization by a #2 bond (1.21 Å): experimental C $\equiv$ N bond length, 1.14 Å. The second #17 atom is used as the  $sp$  nitrogen atom (N#17).

## 8. Sulfur Compounds

As an example of sulfur compounds, the molecule of dimethyl sulfoxide was selected as shown in **Figure 21**, where a pink sulfur atom (S#7) is connected to two  $sp^3$  carbon atoms of the methyl groups by #7 bonds (1.80 Å): experimental C-S bond length, 1.81 Å. The sulfur atom is connected also to an oxygen atom (O#4) by a #6 bond (1.54 Å): experimental bond length, 1.50 Å. It should be noted that the sulfur atom takes the tetrahedral  $sp^3$  configuration, and therefore, the oxygen atom deviates from the C-S-C plane.

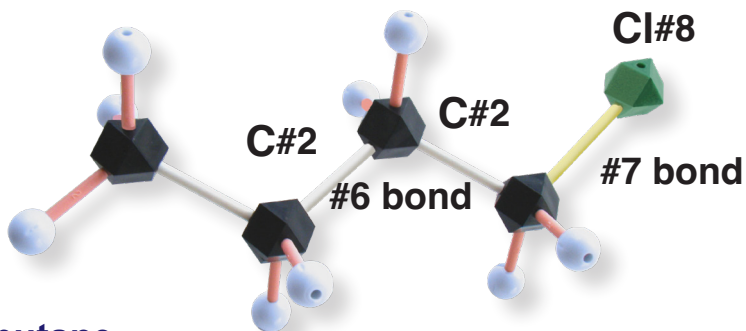
**Figure 21**  
Molecular model of dimethyl sulfoxide



## 9. Halogen Compounds

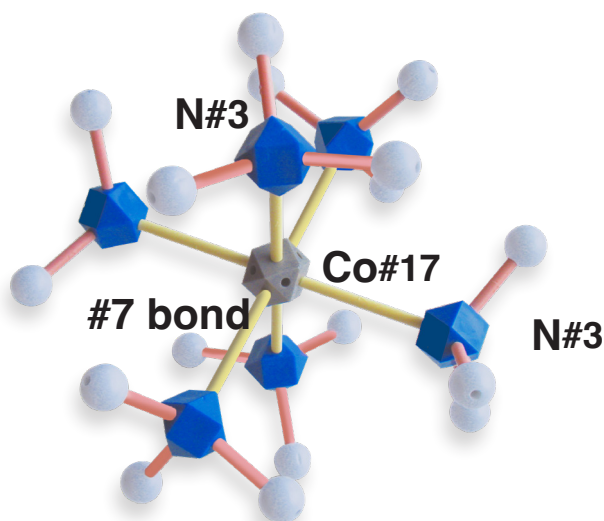
As an example of halogen compounds, the molecular model of 1-chlorobutane is shown in **Figure 22**, where a green chlorine atom (Cl#8) is connected to the  $sp^3$  carbon atom of the butyl group by a #7 bond (1.80 Å): experimental C-Cl bond length, 1.79 Å.

**Figure 22**  
Molecular model of 1-chlorobutane



## 10. Metal Coordination Complexes

As an example of metal coordination complexes, the molecular model of  $[\text{Co}(\text{NH}_3)_6]^{3+}$  ion is shown in **Figure 23**, where a gray metal atom (Co#17) with the  $d^2sp^3$  hybridization is connected to six  $sp^3$  nitrogen atoms of ammonia by #7 bonds (1.80 Å): experimental Co-N bond length, 1.97 Å. This is a typical example of octahedral metal coordination complexes.



**Figure 23**  
Molecular model of a metal coordination complex ion,  
 $[\text{Co}(\text{NH}_3)_6]^{3+}$

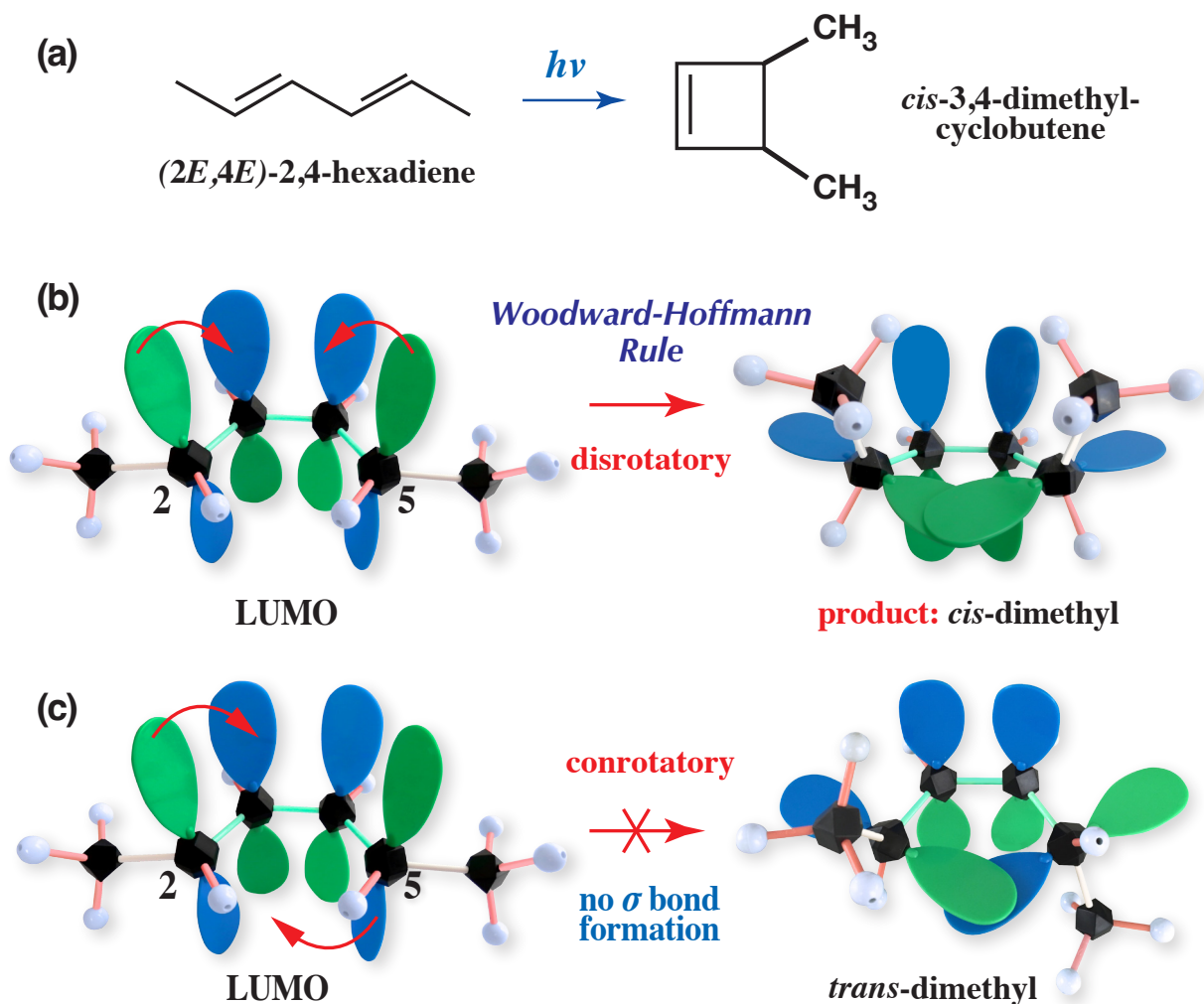
## 11. Woodward-Hoffmann Rule and Fukui Frontier Orbital Theory

As shown in the section of alkene and aromatic compounds, one of the advantages of the HGS polyhedron models is that  $\pi$ -molecular orbitals ( $\pi$ -MOs) can be expressed by  $p$ -atomic orbital ( $p$ -AO) plates. Therefore, the  $p$ -AO plates are useful for demonstrating the Woodward-Hoffmann rule as shown in **Figure 24**, where the rule is applied to the photochemical cyclization of (2*E*,4*E*)-2,4-hexadiene. As shown in **Figure 24** (a), *cis*-3,4-dimethylcyclobutene is formed from (2*E*,4*E*)-2,4-hexadiene under the irradiation of UV light. The mechanism of this reaction is explained by the Woodward-Hoffmann rule as follows.

(2*E*,4*E*)-2,4-Hexadiene is brought by UV light to the electronically excited state,

where the LUMO (lowest unoccupied MO) is expressed as shown in **Figure 24** (b); the green and blue plates indicate the plus and minus signs of  $p$ -AOs, respectively. If two groups including  $p$ -AO plates at 2- and 5-positions rotate in a disrotatory manner, two green plates overlap with each other, and hence a new  $\sigma$  bond is formed making a cyclobutene ring, where two methyl groups take a *cis*-configuration (**Figure 24** (b)).

If two groups at 2- and 5-positions rotate in a conrotatory manner, two methyl groups take a *trans*-configuration in the product as shown in **Figure 24** (c). However, green and blue plates of opposite signs overlap with each other, indicating that a repulsive force exists between them. Therefore, a new  $\sigma$  bond for making the cyclobutene ring cannot be formed. Thus, the reaction with conrotatory motion does not proceed at all; only the disrotatory motion takes place in the reaction.



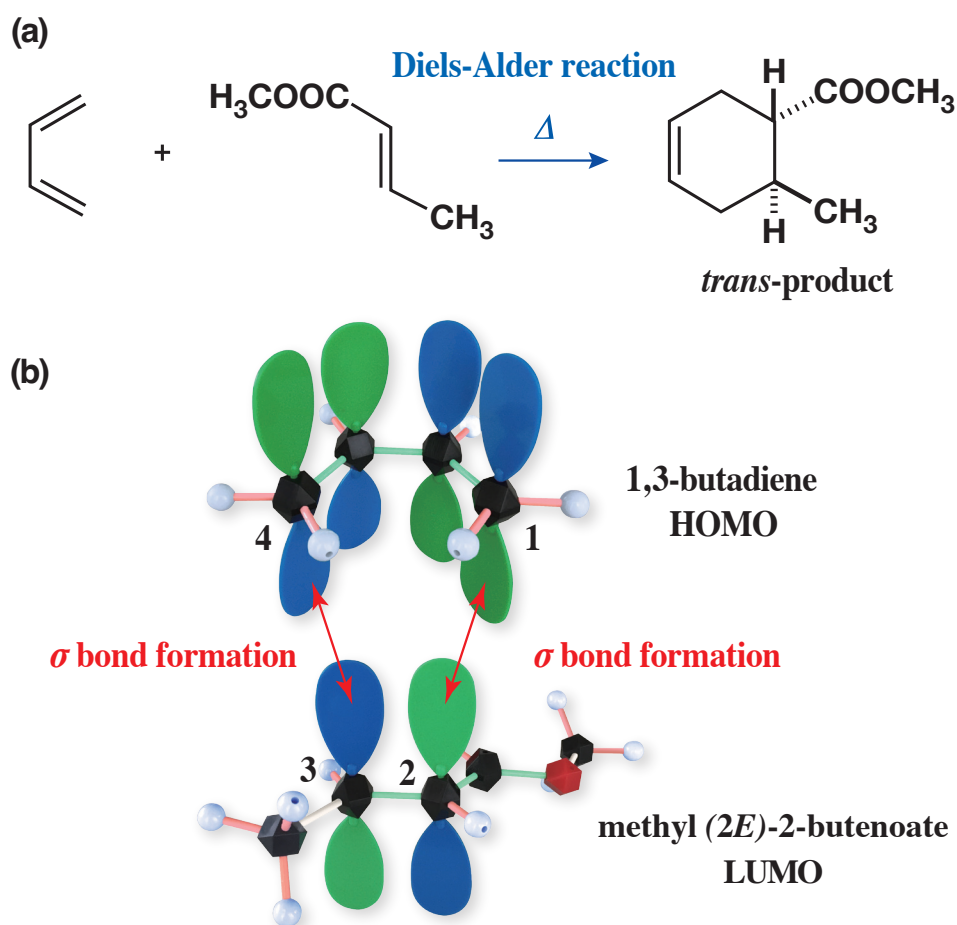
**Figure 24**  
Woodward-Hoffmann rule applied to the photochemical cyclization



In conclusion, the final product takes a *cis*-dimethyl configuration. This is the outline of the Woodward-Hoffmann rule, which is easily explained by using *p*-AO plates.

Next, let's apply the Fukui frontier orbital theory to the Diels-Alder reaction as exemplified in **Figure 25** (a), where 1,3-butadiene is heated with methyl (*2E*)-2-butenoate to form a cyclization product with a *trans*-configuration.

According to the Fukui frontier orbital theory, the HOMO (highest occupied MO) of 1,3-butadiene interacts with the LUMO of the C=C double bond in methyl (*2E*)-2-butenoate, as shown in **Figure 25** (b), where the green orbital plate at the position 1 of butadiene is approaching the green orbital plate at the position 2 of the ester. Because of the same color or sign of the atomic orbitals, this interaction leads to the  $\sigma$  bond formation. Similarly, the blue orbital plate at the position 4 of butadiene is approaching the blue orbital plate at the position 3 of methyl (*2E*)-2-butenoate, and hence another new  $\sigma$  bond is formed. So, a cyclohexene ring is formed.



**Figure 25**  
Fukui frontier orbital theory applied to Diels-Alder reaction

By looking at the molecular model, it is clear that in the final product, methyl and ester groups take a *trans*-configuration. The stereochemistry of the Diels-Alder reaction is explained by the Fukui frontier orbital theory, and its mechanism is thus easily understandable by using the HGS molecular model including *p*-AO plates.

## In Conclusion:

The HGS polyhedron molecular models are thus very useful for students to understand not only molecular structures but also atom hybrid orbital, bond angle, and bond length. Therefore, the HGS polyhedron model is one of the best molecular models and excellent for use by students and researchers. Especially the kits **1013 $\alpha$**  (Organic Chemistry Set for Student), **1003 $\alpha$**  (Organic Chemistry Basic Set), and **1005 $\alpha$**  (Organic Chemistry Standard Set) are highly recommended. Please visit our website,

**<https://hgs.maruzen.info/>**  
**Email: [hgshelp@maruzen.info](mailto:hgshelp@maruzen.info)**



## Important Notice:

With a new manufacturer and improved production process, our polyhedron model sets have upgraded to the new “ $\alpha$  (Alpha)” series. Please be advised that these new sets are only compatible with each other: #1000 $\alpha$ , #1001 $\alpha$ , #1002 $\alpha$ , #1003 $\alpha$ , #1005 $\alpha$ , #1013 $\alpha$ , #1013S $\alpha$ . They are 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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