

# Instruction Manual

# FRAMEWORK MOLECULAR MODELS

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### COMPONENT PARTS OF THE MODELS

The FMM Set is composed of two basic construction units: metal "valence clusters" and plastic tubing by means of which all atoms of the periodic chart can be represented. Each type of unit is color-coded. For example, red tubing represents oxygen, white is hydrogen, blue is nitrogen, black is carbon, etc. Valence clusters are colored silver, brass, and copper for easy identification and fast selection.

Each valence cluster has metal prongs joined end-on at a common point representing the center of the atom. These prongs, which fit snugly into the plastic tubing, point along the symmetry axes of the valence orbitals, and the angles formed determine bond angles in the assembled models.

With the three main types of valence clusters supplied tetrahedron, trigonal bipyramid, and octahedron—you can represent all atoms having up to 12 electrons in their valence shells.

Framework molecular models built from the FMM set show to scale the mutual relations of atoms of a given molecule. The molecular framework is specified by two parameters: One, the internuclear distances measuring the separation between the centers of two neighboring atoms and, two, the bond angles which measure whether two atoms both bonded to a third are

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### **VALENCE CLUSTERS**

The TETRAHEDRON (Figure 1) is used for representation of saturated atoms with eight electrons in their valence shell (sp $^{\rm s}$ 

hybridization—valence angles near 109°), e.g. carbon in alkanes; oxygen in water, alcohols and ethers; nitrogen in ammonia and in alkyl amines.

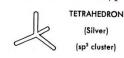


Figure 1

The TRIGONAL BIPYRA-MID (Figure 2) serves a dual function and is employed for: TRIGONAL BIPYRAMID

(Brass)

(sp² cluster)

- 1. Atoms engaged in  $\pi$ -bonds (sp² hybridization)—bond angles at 120° as in C=C, C=O, C=N and also in polynuclear  $\pi$ -orbitals; for example, in benzene ( $C_nH_n$ ).
- Atoms with 10 electrons in their valence shell (dsp³ hybridization—bond angles 90° and 120°); for example, phosphorus in PC1<sub>5</sub>, chlorine in C1F<sub>3</sub>, and tellurium in TeC1<sub>4</sub>.

The OCTAHEDRON (Figure 3) also has a two-fold use:

 For atoms participating in two separate bonds (sp hybridization-bond angles near 180°); for example, the co-linear or bent-out, and if bent-out, to what degree. Take methane as an example (See Figure 10). The points H and C are the centers of hydrogen and carbon respectively and the distance between them is called the internuclear (or interatomic) distance. This distance can be conveniently thought of as composed of two parts the C-x distance measuring the size of carbon in the direction of the bond and known as the covalent radius of carbon; the other (x to H) distance 0.3Å called the covalent radius of hydrogen (See table of covalent radii p. 6). The angle sustained by the

methylene group CH<sub>2</sub> measures about 109° and is called the tetrahedral angle. The angles encountered in the geometry of most molecules are 90°, 109°, 120°, and 180° and are a part of the structure of the three valence clusters provided by the FMM set.

When molecules aggregate to form a crystal or when they collide together at moderate speed their closest contact occurs at a distance corresponding to the van der Waals' envelope which denotes how far the atoms within a molecule extend in the outward direction into space. It is therefore useful to know a third parameter which measures the size of the atom in the non-bonded direction and which is known as the van der Waals' radius of that atom. (A table of van der Waals' radii is given in Table III, p. 7.) Again using the axes of the C—H bond as an example (See Fig. 9), the distance C—x denotes the covalent radius of carbon (black-tubing) the distance x—H denotes the covalent radius of H(0.30Å), and the section H to W extending in the non-bonded direction corresponds to the van der Waals' radius of hydrogen (1.20Å).

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carbon atoms in acetylene ( $HC \equiv CH$ ) or the middle carbon atom in allene ( $H_2C = C = CH_2$ ).

For atoms with 12 electrons in their valence shell (d<sup>2</sup>sp<sup>8</sup> hybridization—bond angles at 90°); for example, iodine in IF<sub>5</sub>, sulfur in SF<sub>6</sub>, and phosphorus in PCl<sub>6</sub>.

The LINEAR FASTENER (Figure 4) is used to join two pieces of tubing to show bonds between unlike atoms, with correct covalent and van der Waals' radii. (Use shown in Figures 8 and 9.)

The ANGULAR FASTENER (Figure 5) is used in the construction of frames, representing  $\pi$ -bonds; for example, acetylene and ethylene.

Figure 5

### PLASTIC TUBING

The chart on the back of this instruction manual shows the two types of tubing that are supplied for the preparation of bonds: solid-color tubing for bonds between like atoms and two-color tubing for bonds joining different atoms.

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The tubing is color-coded as shown in Table I.

### Table I—COLOR CODING OF ATOMS

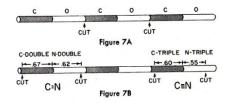
- Hydroger	n-white	Bromine	-orange
- Carbon	-black	Iodine	-brown
- Nitrogen	-blue	Silicon	-light yellow
Oxygen	-red	Phosphorus	
Fluorine	-light green	Sulfur	-dark yellow
Chlorine	-dark green	Metallic ele	

Table II—A	TOMIC	COVALENT RAI	N III
C-single	0.77	Single-l	ond radii
C-double C-triple	0.67 0.60	H	0.30 0.64
N-single N-double	$0.74 \\ 0.62$	Si P	1.17 1.10
N-triple	0.55	S C1	1.04 1.00
O-single	0.74	Br	1.14
O-double	0.62	I	1.33
O-triple	0.55		

A particular atom is identified by means of the color, and its covalent and van der Waals' radii are given by the length of the section of the tubing. This means that both the size of the atom

Figure 6

colors. (See back cover.) Three bonds can be obtained from each piece of tubing, as shown in Figure 7A. Double and triple bonds, being shorter than single bonds, can be cut accurately from the same type of tubing, as shown in Figure 7B, using the values of covalent radii from Table II.



### **Bonds Between Like Atoms**

DECIMAL INCH SCALE Double the value of covalent radii (Table II, p. 6) for bonds between like atoms (i.e., C-C, single bond 2 x 0.77=1.54, and C=C double bond 2 x 0.67=1.34).

and its position are made clearly visible within the framework of the molecule.

Twelve colors are provided (Table I), and sections are cut from these on the relative scale of 1A = 1 inch, as specified by Tables II and III, which list the covalent and van der Waals' radii of the most common atoms.

	Table III—VAN	DER	WAALS'	RADII	IN Å*		
N	1.5	0	1.40		Н	1.2	
P	1.9	S	1.85		$\mathbf{F}$	1.35	
As	2.0	Se	2.00		C1	1.80	
Sb	2.20	Te	2.20		Br	1.95	
					I	2.15	

Note: The van der Waals' radius is approximately 0.80 to 0.90 Å larger than the covalent radius. The thickness of the aromatic molecule is 3.20 Å.

### CONSTRUCTION OF BONDS

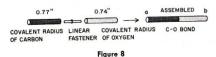
Bonds between like atoms are cut from tubing of one color; 1½ inch sections approximate the relative bond lengths between light elements (i.e., C-C, N-N, O-O). More accurate bond lengths can be cut by using Tables I and II and the decimal inch scale provided in the inside of the box, as shown in Figure 6.

Single bond distances between different atoms are obtained by cutting the striped tubing at the interface between two

### C-O Bond

C-H Bond

A section of black tubing 0.77 inches long (covalent radius of carbon 0.77Å) is attached to a 0.74 inch section of red tubing (covalent radius of oxygen 0.74Å) by means of a linear fastener, to form the carbon-oxygen bond, as shown in Figure 8.



A 0.77" section of black tubing representing the covalent radius of carbon is attached by means of a linear fastener to a white section of tubing 1.5" long, which represents the diameter of the hydrogen atom measured along its axis of symmetry, and is the sum of the covalent radius of hydrogen 0.30" toward the carbon and the van der Waals' radius of hydrogen 1.20" away from carbon, as shown in Figure 9. ASSEMBLED

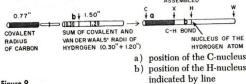


Figure 9

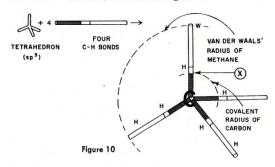
123456789 12345678921234567893123456789

### CONSTRUCTION OF REPRESENTATIVE STRUCTURES

A great variety of molecular structures can be depicted with the FMM Set. You can represent any atom up to and including six bonds—thereby permitting you to construct most known molecules. The ease of construction of molecular models is shown by the following representative structures.

### I. METHANE (CH<sub>4</sub>)

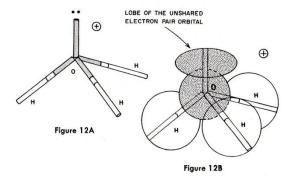
The methane molecule is quickly built from a tetrahedron and four C—H bonds, as shown in Figure 10.



C) position of the C-nucleus

H) position of the H-nucleus

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major and a minor one. The smaller of the two is located within the general sphere defined by the covalent radius of the oxygen atom and, therefore, only the major lobe of the unshared pair electron orbital is shown.

## III. METHANOL (CH3OH)

The model of methanol is constructed in two steps:

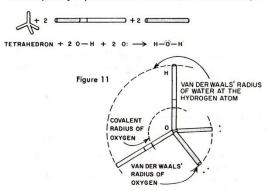
 The building of the C—OH skeleton. The carbon tetrahedron is attached by means of a C—O bond to an oxygen tetrahedron, which in turn carries an O—H bond, as shown in Figure 13.

### II. WATER AND HYDRONIUM ION (H2O, H3O+)

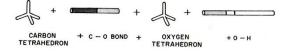
The water molecule (Figure 11) is constructed by attaching two O—H bonds and two sections of red tubing to a tetrahedral valence cluster.

The hydronium, H<sub>3</sub>O<sup>+</sup> (Figure 12A) is formed by exchanging one unshared electron pair axis for an O—H bond. The relationship of the axis of the remaining unshared electron pair orbital to its three-dimensional shape is shown in Figure 12B.

The orbitals traced out by the unshared pair of electrons is essentially an sp<sup>a</sup> hybrid orbital and as such has two lobes; a



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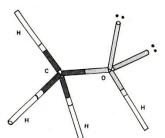


Figure 14

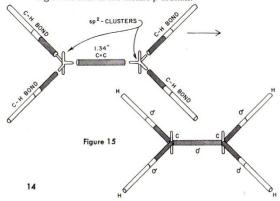
 The model is completed by attaching three C—H bonds to carbon, and pieces of tubing (1.4 inches equaling van der Waals' radius of oxygen) representing the symmetry axes of the two unshared electron pair orbitals of oxygen.

### IV. ETHYLENE (CH2=CH2)

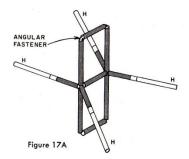
The two carbons of ethylene are both in the sp² hybrid state and are represented by trigonal bipyramids. The construction is accomplished in three steps:

1. Construction of the planar sigma bonds framework:

The trigonal bipyramids can be considered to have two types of prongs: (a) three prongs lying in a plane all  $120^{\circ}$  apart (hereafter called the  $\mathrm{sp^2}$ -prongs)—these engage in sigma orbitals or unshared electron pair orbitals—all of which are situated in a single plane; and (b) the other perpendicular prongs (the atomic p-orbital prongs) are used for attaching of the axes of the atomic p-orbitals.



Waals' distance with right angle fasteners, as shown in Figure 17A. The relationship of the frame to the space-filling form of the  $\pi$ -orbital is indicated in Figure 17B.



Note that with the completed  $\pi$ -orbital frame, rotation about the C-C bond is more restricted, consistent with the known geometry of ethylene.

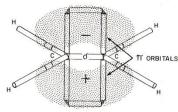
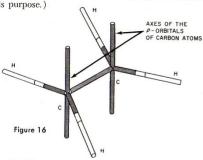


Figure 17B

Two trigonal bipyramids of the two carbons are attached at the  ${\rm sp^2}$ -prongs by means of a section of tubing 1.34" long (see Table II). The four C—H bonds complete the planar assembly of atoms held together by sigma-bonds, as shown in Figure 15.

2. The axes of the atomic p-orbitals centered on the carbons is shown in Figure 16 by means of sections of tubing attached to the two remaining atomic p-orbital prongs on each trigonal bipyramid. These sections of tubing are 1.54" long, giving an effective length of 3.08Å, corresponding closely to the van der Waals diameter of the π-bond. (Single C—C bonds have appropriate lengths for this purpose.)



3. The  $\pi$ -orbital frame is completed by means of two sections of black tubing (0.67" long) attached at the van der

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## V. FORMALDEHYDE (CH2O)

The same sequence of steps is taken for the construction of formaldehyde with the difference that two-color tubing is used to distinguish oxygen from carbon, and axes of unshared pairs

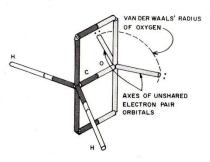


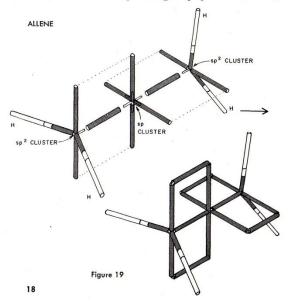
Figure 18

on oxygen are indicated by sections of red tubing, as shown in Figure 18.

### VI. ALLENE (CH2=C=CH2)

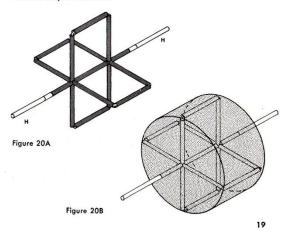
The terminal  $CH_2$  groups of allene are constructed in the same manner as the carbon atoms of ethylene. The two  $CH_2$ =

units are attached (as indicated by dotted lines in Figure 19) to the central carbon atom, represented as an octahedron (sp hybridization) by sections of tubing representing two sigma bonds, and two frames representing two perpendicular  $\pi$ -bonds,



### VII. ACETYLENE (HC=CH)

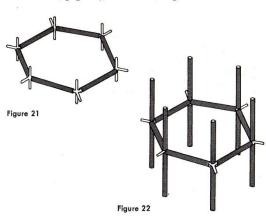
The two carbon atoms of acetylene (octahedral clusters) are attached by one section of tubing representing a sigma bond and two perpendicular frames of the two  $\pi$ -bonds, as shown in Figure 16. It is believed that acetylene actually has cylindrical symmetry and that the two  $\pi$ -orbitals are indistinguishable–representing a unified cylinder as indicated in Figure 20B. The  $\cdots$ C $\equiv$ N;  $\cdots$ N $\equiv$ C:,  $\cdots$ C $\equiv$ O: $^\oplus$ , and  $\cdots$ N $\equiv$ N: $^\oplus$  groups are similarly constructed.



### VIII. BENZENE (C6H6)

The benzene molecule is constructed in three steps:

- Six trigonal bipyramids are connected by means of six C—C bonds into a sigma-bonded frame, as shown in Figure 21.
- The atomic p-orbitals are erected on all the trigonal bipyramids in a manner analogous to ethylene (see Section IV, page 14), as shown in Figure 22.



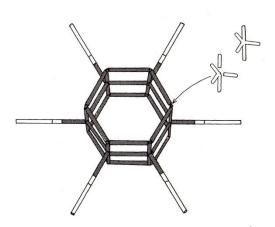


Figure 23

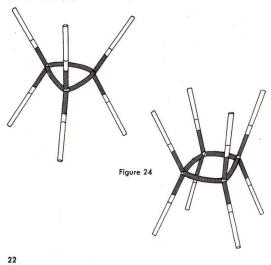
The atomic p-orbitals are connected at the ends by means
of trigonal bipyramids, whose two unused prongs were
broken off, as shown in Figure 23. Six C—H bonds complete the framework of benzene.

Models of pyridine ( $C_sH_sN$ ), furane ( $C_4H_4O$ ), tropylium ion ( $C_7H_7^{\oplus}$ ), etc., are assembled in an analogous manner.

### SPECIAL CONSTRUCTION PROBLEMS

### **Small Strained Rings**

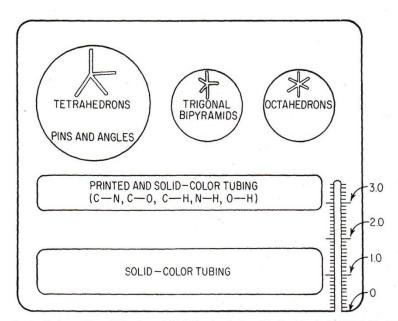
Three- and four-membered rings are built without difficulty by means of the flexible tubing provided. Models of cyclopropane and cyclobutane (Figure 24) illustrate this unique feature of the FMM Set.



# FMM STUDENT KIT COMPONENT LIST

### **Metal Components**

Angle																												
Octahedron				8				100					ī		7												3	10
Trigonal Bipyramid																												18
Tetrahedron																										*		30
Pins														\$0 \$0														10
Tubing																												
Light Green (F)	24									2						100	27.	90%		2		٠	20	7	72		100	2
Dark Green (C1)					200																							2
Orange (Br)													88					-		8	ಿ					*	*	2
Brown (I)									•		•	•	*	•														0
Violet (P)																												
Light Yellow (Si)				•														- 2		•								0
Dork Vollow (S)										٠														•			*	0
Dark Yellow (S)							:	-		٠	*	1						ä		*				٠	*	٠	*	2
Gray (Metals)			•	7			100	5		٠								8			٠	٠	*			٠		2
White (H)			*	*	,					٠					. ,			ÿ									٠	6
Black (C)																											. 2	23
Blue (N)					970																							4
Red (O)																											. 1	10
Red-White (O-H)			100				-											÷										3
Blue-White (N-H)		-	200																									3
Black-White (C-H)																	000											20
Black-Blue (C-N)	1707		 200			•				•			•						•									5
Black-Red (C-O)													•						•									5



Parts Sales: ChemKits, Inc. 2124 Simbrah Dr., Cedar Park, TX 78613-1303 http://www.chemkitsinc.com (email: tjempty@chemkitsinc.com)