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INORGANIC CHEMISTRY SERIES

Set NS-01B

A

This Set Contains:

Made in the Philippines © 2015 KitaMo Molecular Models

Octahedral *16	6 Gray			
octaneural	2 Brown 1 Yellow 1 Violet			
Trigonal	6 Dark Gray			
Bipyramidal "16	2 Brown 1 Yellow 1 Violet			
Tetrahedral *16	6 Black 4 Blue 2 Red			
reuaneurai	2 Brown 1 Yellow 1 Violet			
Bent <sup>*16</sup>	4 Red			
Monovalent "12	14 White 6 Green			
wonovalent	4 Orange. 4 Purple			
	12 14-mm Straight			
Links	12 19-mm Straignt			
LINKS	12 27-mm Bent			
	100 cm Uncut Link Material			

Bead diameter in millimeters

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# **KITAMO MOLECULAR MODELS INORGANIC CHEMISTRY SERIES** Set No. NS-01

The KitaMo Molecular Models Set No. NS-01 is designed for the construction of ball-and-stick molecular models using octahedral, trigonal bipyramidal, tetrahedral, bent and monovalent atoms and their derivatives (e.g., square planar, trigonal planar and linear). The links for making bonds, given their fixed lengths, yield models of various scales. Uncut link material is included for the preparation of additional links.

### Set Contents

	Octahedral	Trigonal Bipyramidal	Tetrahedral	Bent	Usage (See Note 2)
Gray	6				Metal
Dark Gray		6			Metal
Black			6		Carbon
Blue			4		Nitrogen
Red			2	4	Oxygen
Yellow	1	1	1		Sulfur
Violet	1	1	1		Phosphorus
Brown	2	2	2		Metal

11111		± 1	nyarogen		
Green		6	Halogens		
Orange		4	Bromine		
Purple		4	Iodine		
Links			Usage		
12	14 mm	Straight	Single Bonds		
			SINGLE BONDS		

100 cm Uncut Link Material

19 mm Straight

27 mm Bent

14

Monovalent

White

12

12

1

Notes: 1. Bead Diameters: Monovalents 12 mm; All others 16 mm.

2. Suggested Usage. Color assignment is user-specified.

The set is packaged in a plastic case.

The colored pictures on the case cover are described in the discussion below (referred to as Figures). Some of the models shown are for illustrative purposes only and cannot be exactly reproduced using the parts in this set.

## Atoms

Atoms are represented by colored polyurethane beads with at least one hole. The holes are designed for 2.0 mm diameter links with an insertion depth of 4.0 mm. Each hole has a PVC insert which holds the link in place and allows for bond rotation.

### **Bonds**

Bonds are made using straight and bent nylon links. Other link materials can also be used (see discussion below).

Cutting the link material. A utility knife or blade held at the correct angle makes clean and straight cuts, however blades may be inconvenient to use. Diagonal wire cutters or similar tools (e.g., nail nippers) offer more convenience but with cut deformities due to the indenting/wedging action. Scissors tend to deform the most due to the shearing action.

Bent link preparation. Cut the link to length, hold it lengthwise with one hand between the thumb and forefinger and bend it while guiding the center bend with other hand. The material tends to curl, so it is best to bend in the direction of the curl.

## **Bonds Using Straight Links**

The 14 mm and 19 mm straight links are based on the lengths of C-H (1.09 Å) and C-C (1.54 Å) single bonds, respectively. When used to model such bonds, the resulting scale is about 1.7 centimeters per Angstrom (cm/Å). Using these links for other bonds may result in models with different scales. For example, all the models in Figure D are made using 14 mm and 19 mm straight links. Assuming none of them has C-H and C-C bonds, then each model shown has a scale different from 1.7 cm/Å.

The slightly flexible straight links allow for angular variations and can be used for strained bonds. The rightmost model in *Figure D* represents cyclopropane ( $C_3H_6$ ), a molecule with highly-strained bonds.



Usage

(See Note 2)

Hydrogen

Double / Triple

Bonds

#### Bonds Using Bent Links: Multiple Bonds

The 27 mm bent links are used for double and triple bonds. When used to model C=C double bonds (1.34 Å), the scale is approximately 1.7 cm/Å. For double bonds involving other atoms, or for triple bonds, the resulting scale may be different. *Figure B* shows models with multiple bonds. The ethynylbenzene ( $C_8H_6$ ) model on the left has double and triple bonds, all modeled using bent links.

To assemble multiple bonds, first insert all the bent links into one bead only. Then insert the free ends of the links into the second bead one at a time. Holding the assembly against a hard surface bends the link at a convenient angle and helps during link insertion.

When bent links are used to model a multiple bond, the number of bent links is equal to the bond multiplicity. While such a representation clearly distinguishes between double and triple bonds, the multiple bond lacks the sigma bond portion and does not accurately show the pi bond structure. An alternate representation may be made by using other shapes which are more appropriate based on theory. For example, at the top right of *Figure B* is a model of ethylene ( $C_2H_4$ ) that does not use tetrahedral ( $sp^3$ ) carbons and bent links. Instead, trigonal ( $sp^2$ ) carbons and straight links are used. The sigma bond portion of the double bond is represented by a 16 mm straight link, while each half of the pi bond (i.e., one lobe) is made up of two 14 mm links with the free ends linked by a small rubber band (not supplied).

#### Scale

The scale of a model is determined by the lengths of its links (i.e., a model with a specific scale can be made using links cut to the appropriate lengths). Given the fixed bead diameters, the atoms/ions they represent are not to scale in most cases.

Using the supplied pre-cut links for different molecules may result in scale variations as discussed above for *Figure D*. There are times when scale is insignificant, but it may help to make models to scale in certain cases. For example, in a model where the bond lengths involved vary significantly; or when the relative sizes of two molecules are being considered.

<u>Figure A</u> shows three models all made to a scale of about 1.3 cm/Å using a variety of link materials (see discussion about link materials below). Clockwise from top: Cobalt complex ion,  $[Co(NH_3)_5Cl]^{2+}$ ; Sulfur Trioxide (SO<sub>3</sub>); and Sulfur Tetrafluoride (SF<sub>4</sub>). Note that for the complex ion, the lengths of the Co-Cl, Co-N and N-H bonds are all different. Note also the use of a link to represent the lone pair in the seesaw structure of SF<sub>4</sub>. *Color code: Co brown; Cl green; N blue; H white; S yellow; O red; F green.* 

<u>Figure C</u> shows Silicon Carbide (SiC) and Zinc Blende (ZnS) models also made to a scale of about 1.3 cm/Å. Both are diamond-type networks, but the unit cell of SiC is smaller compared to that of ZnS. *Color code: C black; Si brown; Zn violet; S yellow*.

The minimum scale is achieved by using 8 mm straight links (not supplied), resulting in models where the bead surfaces touch (i.e., no part of the link is visible). For example, the complex ion in *Figure A* has five NH<sub>3</sub> structures with 8 mm links used for the N-H bonds. In some cases, using only 8 mm links result in structures that approximate the appearance of space-filling models.

**Note:** The nylon link material may be difficult to use in larger scales (it is supplied in rolls, hence the tendency to curl). In such cases, straight rigid materials may be necessary (see discussion about link materials below). However, for larger scale models with multiple bonds, the curling tendency of the nylon material may be favorable, and may eliminate the need for bent links.

### **Using Other Link Materials**

Links other than those supplied with the set can be made by using a variety of readily-available materials (e.g., toothpicks, wooden dowels/applicator sticks, plastic/metal rods and flexible plastic tubing). Given this choice of materials, models of various scales and appearances may be constructed. While the preferred cross-section for the links is circular with a diameter of 2.0 to 2.3 mm, other geometries may also be practical.

In *Figure A*, the two-color links are made from toothpicks cut to the appropriate lengths and colored with ink markers. In *Figure C*, the SiC model uses plain toothpick links while the ZnS model uses colored toothpicks.

Practical issues must be considered when using other link materials (e.g., toothpick diameter variations). Please visit our website (kitamomolecularmodels.com) for model making hints and tips.