KitaMo Molecular Models

Design Guide for Custom-Made Molecular Models

(Edition 2.0)

This Guide is intended to help model users prepare the specifications for custom-made ball-and-stick molecular models.

If your requirements are not discussed in this guide, please submit an inquiry to:
inquiry@kitamomolecularmodels.com.

WARNING:

KitaMo Molecular Models are NOT TOYS.
Allow children to handle them only with close adult supervision.
They are built with structural integrity but can easily be damaged by mishandling.

Do not quench your inspiration and your imagination;
do not become the slave of your model.
Vincent Van Gogh

KitaMo Custom-Made Molecular Models are permanent "ball-and-stick" physical representations of molecules.

The materials used are quite ordinary: plastic beads (the "atoms/ions") and steel wire (the "bonds"). With thoughtful design, precisely-machined parts and meticulous assembly, tactile three-dimensional representations of chemical structures are constructed.

The models are typically built to a compact scale of 1 centimeter per Angstrom (100 million times actual size). At this scale, the miniature models allow for easy handling and viewing, and require minimal display space.

The tools and techniques used to produce the miniatures may be adapted to build larger scale models, not only for chemistry, but for other applications where tactile ball-and-stick structures are essential.

NOTE: **Model construction cannot be rushed**.
It requires careful planning and many of the construction methods are labor-intensive.

Specifications Checklist	***Molecule Name/Formula***	***Accuracy***
The following must be specified	***Structure***	***Display Preference***
for a custom-made molecular model:	***Scale***	***User Assembly***
	Color Scheme	***Cosmetics***

Molecule Name and Formula

It is important that the actual molecule be distinctly identified by specifying the structural formula, chemical name and common name(s). Names are critical especially for polymorphic molecules. For example, ZnS may either be wurtzite or sphalerite (zincblende).

Structure.

Given a structural database, the number of atoms, the number of bonds, the bond angles and the bond lengths can all be determined. Structural information is best specified using atomic coordinates and bonding interactions. There are several popular electronic formats for this purpose. The preferred format is PDB.

It is important that the structural information be submitted in its final form, giving a clear and complete description of the finished structure. Partial and incomplete information require further processing that may result in errors. Crystal symmetry data may be helpful, but is not necessary.

For very simple models, a drawing with ALL the necessary dimensions may be sufficient.

Scale

The scale relates the size of the physical model (in centimeters) to the actual molecular dimensions (in Angstroms). While any units of length are acceptable, the units just mentioned are preferred and the scale is specified in ***centimeters per Angstrom (cm/Å).*** Given the scale, the actual dimensions of the finished model can be determined.

Instead of specifying the scale, an alternative is to specify two dimensions: (1) a target dimension for the physical model (in centimeters) and; (2) its corresponding molecular dimension (in Angstroms). The ratio of these two corresponding dimensions gives the scale of the model.

NOTE: **Consider a uniform scale when planning a collection of models.**
Often, the primary purpose of the model is to show structure, and for an individual or isolated model, the scale may not matter significantly. However, when two or more different molecules are involved, models made to the same scale will show their relative dimensions.

Plastic Beads for Atoms and Ions

Colored polystyrene beads, commercially known as "chalk beads", are used to represent the atoms/ions. Holes are drilled into the beads at precise angles and locations.

Bead colors. There is no standard color scheme for molecular models. Color schemes used by some popular models have found widespread acceptance over the years (See Appendix A). The beads are used as supplied and the available colors may not exactly match user requirements.

Bead sizes. Various bead sizes can be used to show the ***relative sizes*** of the atoms/ions. Although desirable, it is often impossible to select bead sizes that are proportional to the model's scale. Available bead diameters are 4, 5, 6, 8, 10, 12 and 16 millimeters. The 4 and 5 mm beads are typically used for hydrogen.

Metal Links for Bonds

Stainless steel wires are used to represent the bonds. It is the wire lengths that determine the scale of the model. The wires are cut to precise lengths, inserted into the bead holes, and fixed permanently in place with epoxy and/or cyanoacrylate adhesive. Available wire diameters are 0.70 mm and 1.10 mm.

By default, only one wire is used to link two beads regardless of the bond order. Additional links may be added to show double and triple bonds.

Models are assembled for static display, with all the parts fixed in place. As an option, single bonds can be allowed to rotate so the model can be displayed in various conformations.

Bond colors. The simplest models are constructed using plain unpolished stainless steel wire. Bond colors can be added to enhance the appearance of the model or to distinguish between bond types (e.g., covalent bonds are colored while hydrogen bonds are bare metal). Color is added by slipping colored vinyl tubing over the wire or by painting.

Available vinyl tubing colors are black, blue, red, yellow, orange, green and white. The vinyl tubing outside diameter is 1.5 mm. Since the vinyl tubing and the bead materials are not the same, color matching cannot be guaranteed.

If bond colors are used, there are two options:
(1) One Color, i.e., using one and the same color for all the bonds;
(2) Two-Color, i.e., each color is inherited from the parent atom, resulting in a demarcation line halfway along the llink.

Ideally, the physical model shows how the molecule is held together by covalent, ionic and/or hydrogen bonds (i.e., each link in the model corresponds to a chemical bond in the molecule). However, certain situations require the use of "imaginary links" which do not correspond to any chemical bonds. This is often done for structural support (without which model construction becomes difficult, if not impossible), or for alignment and display purposes. Imaginary links may look like chemical bonds so the best effort is made to minimize their usage and make their appearance distinct from the chemical bonds.

Accuracy

It is during assembly that the final accuracies are realized. The best achievable tolerances are ± 1 degree for the bond angles and ± 0.5 mm for the bond lengths. For highly symmetrical structures, accuracy is very important.

If the structure allows, the maximum tolerances can be relaxed to ± 3 degrees for the bond angles and ± 1.0 mm for the bond lengths. Relaxed tolerances, if applicable, mean easier construction and lower cost.

Display Preference

The model may or may not require a base/stand or some other mounting method. In certain cases, like the DNA double helix, the stand is required to support the model. Also, to achieve the desired display preference, it may be necessary to add the previously mentioned "imaginary links".

The default stand material is 1/8" thick clear acrylic sheet. Given this clear material, it is possible to pick up the model and view it from the bottom. Please consult KitaMo if a different stand material is required.

User Assembly

In case the model needs to be shipped, it may be advantageous to ship it partially-assembled. The user does the final assembly. This is done to minimize the risk of damage during transit. It also facilitates packaging, which may affect shipping and handling costs. Suggestions are made about the sub-assemblies and are only implemented with the user's final consent.

Cosmetics

While care is taken during construction, cosmetic imperfections may be present in the finished model. These do not affect the structural integrity of the model and in most cases are subtle and almost unnoticeable. Some of these cosmetic imperfections are permanent due to the nature of the materials/methods used:

* Mold marks. Beads always come with a mold parting seam and an injection mark.
* Bead holes. The beads are supplied with an axial hole through the spherical structure. In certain cases, this hole remains evident even if it is filled.
* Color mismatch for two-color bonds. The bead and vinyl tubing are of different materials and no effort is made to match their colors.

If necessary, some of these imperfections can be corrected, at additional cost, to improve the physical appearance of the model (See Appendix B).

Appendix A: The CPK Color Scheme

The CPK Color Scheme is used by CPK molecular models designed by chemists Robert Corey, Linus Pauling and Walter Koltun.

Element	Color
Hydrogen (H)	white
Carbon (C)	black
Nitrogen (N)	dark blue
Oxygen (O)	red
Fluorine (F), Chlorine (Cl)	green
Bromine (Br)	dark red*
iodine (I)	dark violet*
Noble gases (He, Ne, Ar, Xe, Kr)	cyan
Phosphorus (P)	orange
Sulfur (S)	yellow
Boron (B) and most transition metals	peach, salmon
Alkali metals (Li, Na, K, Rb, Cs)	violet
Alkaline earth metals (Be, Mg, Ca, Sr, Ba, Ra)	dark green
Titanium (Ti)	gray*
Iron (Fe)	orange
Other elements	pink

* this color is not available for KitaMo Molecular Models

Appendix B: Correcting Cosmetic Imperfections

Some cosmetic imperfections take time to correct and by default are left uncorrected on the model. These can be corrected, at additional cost, to improve the physical appearance of the model.

Bead Holes. Beads are supplied with an axial hole (about 1.6 mm diameter). Very often, at least one end of the hole is used for bonding. The unused end is kept open, leaving a dimple.
** Remedy: This dimple can be filled with colored resin to improve the spherical surface contour, however perfect color matching between the bead and the resin used for filling cannot be guaranteed.*

Random traces of excess adhesive at bond roots. Adhesive is clear or light tan in color and the best effort is made to minimize adhesive build-up. However some noticeable amount may still be left.
** Remedy: All bond roots are meticulously cleaned up to remove unwanted traces of adhesive.*