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A comparative review of five brands of molecular model kits.
With notes on the educational merits of kits in an age of software.
by David Walker, UK

Brands illustrated – ChemKits, Inc., Minit, Molecular Visions (Darling Models, Inc.), Molymod, Orbit.

Contents:

Molecules in the News [link to separate gallery] illustrated with models both physical and rendered in software, e.g. heptacene - the longest acene synthesized (March 2017), elusive triangulene' synthesized (Feb. 2017), molecular machines (Nobel Prize for Chemistry 2016).

Introduction

I've had a fascination with molecular model kits since using two brands (Orbit and FMM) as a student in the mid 1970s. Despite the now wide availability of molecular modelling / visualisation software on all computer platforms (including smartphones!), there is still much to recommend the hands-on experience of building and studying molecular structures using kits where appropriate. The brands and their kits can differ widely in their construction methods, scale and thus how each represents a molecule. (For a short history of their use, see e.g. Francoeur (1997, ref. 1).

As a project I was interested in how five of the current major brands represented molecules and sharing aspects may be of interest. A features summary for a typical kit of each brand is offered plus illustrations of models for a selection of molecules, from the simple to the more complex. Although it tries to be fairly objective, it remains of course, very much a personal view. Notes through the text on software are highlighted in yellow.

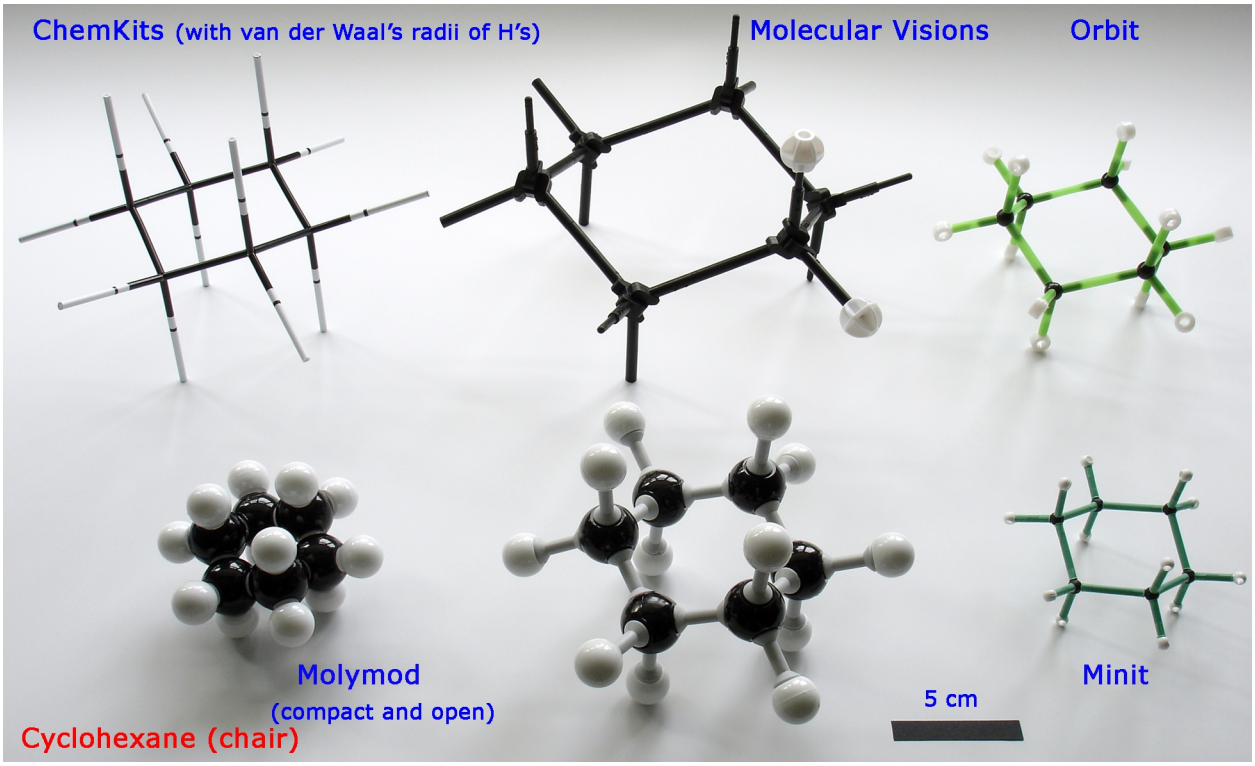
This article concentrates on building organic molecules. Many of the kits or the makers' companion kits are suitable for building inorganic structures, lattices etc. Dedicated kits are also supplied by some. It is hoped to illustrate these type of models in a later part 2.

Brief summary of main molecular model types and some construction approaches (links are to Wikipedia's entries)
Ball and stick model - Atoms and bonds are represented by coloured spheres and rods respectively. Molymod molecules assembled using its 'open' form are of this type. Both this type and the skeletal models are particularly suited to show aspects such as interatomic relationships, bond angles / strain, conformations.
Skeletal model – The atom centre parts do not show atomic radii to any degree and the molecular model uses thin rods to show bonds. ChemKits is the 'purest' form of this type with atomic covalent radii (and van der Waals radii for O-H, N-H) shown in standard colours along a rod. The Minit and Orbit with small coloured atom centres rather than coloured links are also essentially a skeletal type; the Orbit with its larger coloured atom centres showing features of both the skeletal and ball and stick models.
Space-filling model - These are the nearest to representing a molecule's external form by showing van der Waals radii / surfaces (the closest distance two non-bonding atoms / discrete molecules can approach) and especially valuable when studying processes where this aspect is important such as intermolecular interactions. Molymod molecules assembled using its 'compact form' to create 'semi-space-filling' models approach this type.
CPK colours - Model kits typically use a form of the standard CPK colour scheme for each element, either for the atoms and/or the bonds e.g. carbon - black, hydrogen - white, oxygen - red, nitrogen - blue. Some kits use bi-colour bonds between atoms of different elements to show their respective covalent radii.

Depending on what the structure is built to show, it may not be necessary to build the complete molecule, especially if this aids clarity. Examples are provided. Note that some kits are shown in part use by the author and not necessarily as purchased. In some cases I use both my old and new examples of kits. This is noted where necessary. Readers can visit a maker's website to check the kits as supplied and presented when new.

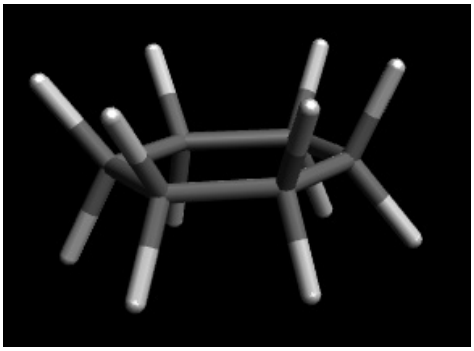
Cyclohexane and benzene

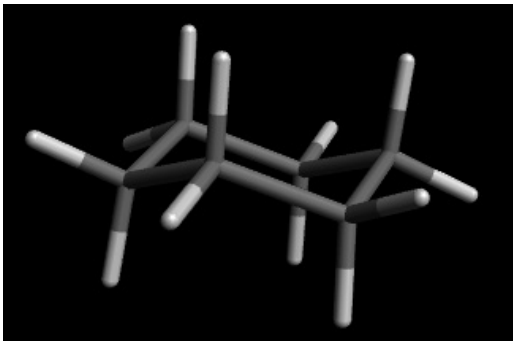
How each kit represents two common molecules, cyclohexane and benzene, are shown below. Cyclohexane is a particularly pertinent example as it shows how using software rather than a physical kit to build the molecule can potentially mislead those unfamiliar with the often complex software programmes available.



Above: Cyclohexane made using the five kits. The black bar is 5 cm (ca. 2 inches) (The Orbit model uses the author's older kit, see below for molecules built using a modern kit.). Also see later the Molymod Molyorbital model of cyclohexane.

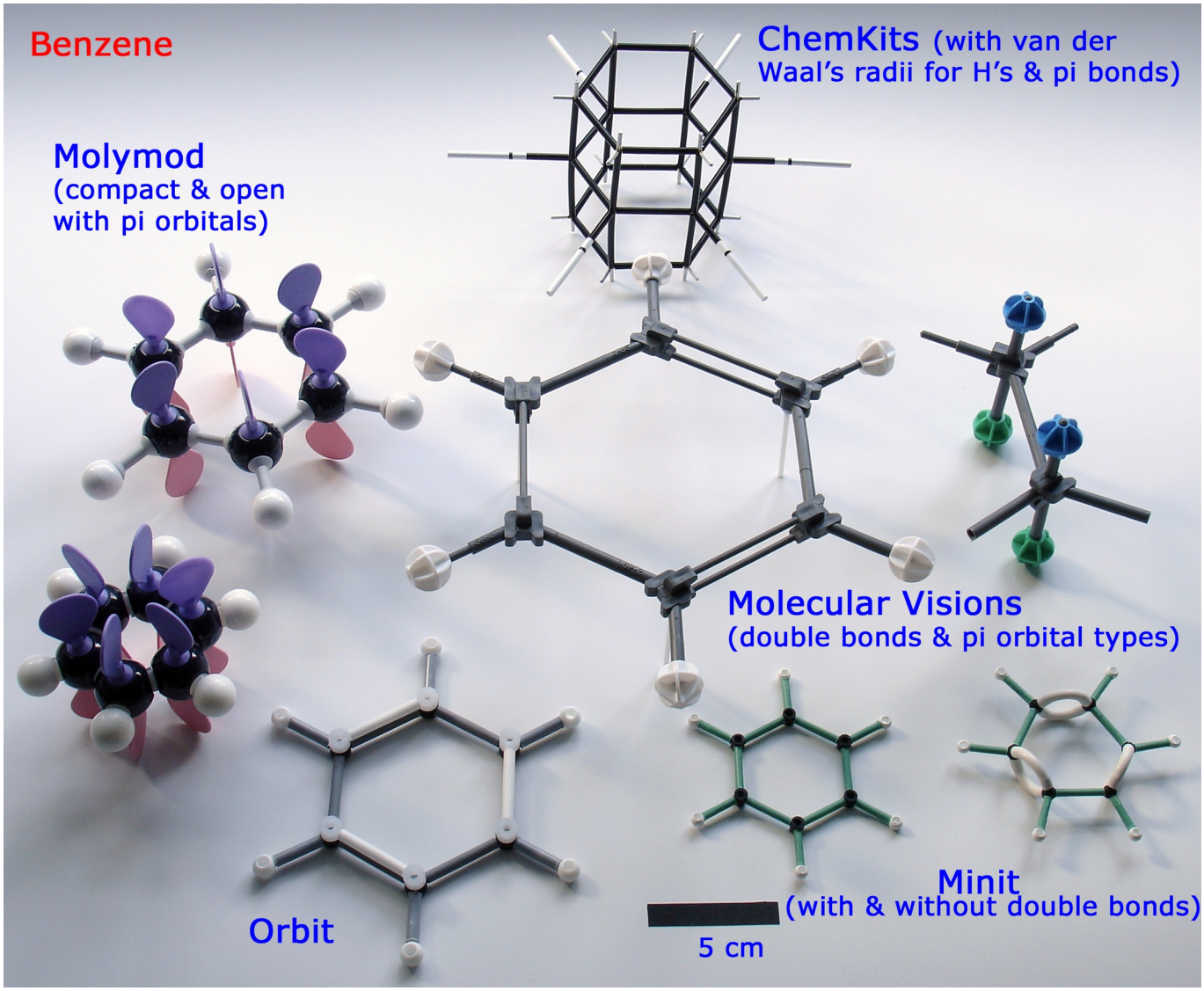
Software note: *A user of a kit to build cyclohexane will immediately appreciate that it does not preferentially adopt a planar form. With some 3D modelling software, although the default option may build a molecule using a 3D perspective it does not show its true structure. The user must become familiar with the software's features to present in its true 3D form.*





Left above. Cyclohexane built using default settings in Avogadro shows the ring as planar. The feature 'Optimise Geometry' in a drop-down 'Extensions' menu has to be activated to show one of its true 3D forms (the chair conformer) as shown right above. (Another software suite tried ACD / ChemSketch is similar.) Arguably, exploring cyclohexane's 'boat' and 'chair' conformers is also better appreciated handling real models, less so manipulating screen images. I haven't yet discovered how to flip between conformers in software.

Addendum. Since completing the article, I've found a programme that does represent drawn molecules such as cyclohexane correctly without the need to manually optimise the geometry. Herman Bergwerf's MolView has a routine to check a molecule's structure on databases before presenting a 2D structural drawing as the 3D molecule. There's no doubt more software examples and arguably the better choice for beginners.



Above: Benzene made using five different kits. The black bar is 5 cm (ca. 2 inches)

Comments: Benzene is a particularly good molecule for showing how each kit can represent double bonds and in some cases the p orbitals and their ability to delocalise. Some standard kits, as well as being able to show the so-called Kekulé forms with localised double bonds can also show localised p orbitals (above, two lefthand Molymod and righthand Molecular Visions models).

ChemKits include angled connectors to represent delocalisation as shown above at the correct van der Waals distance. Supplied angled connectors can also show pi-bonds in molecules such ethene and ethyne.

Molymod also offers a special Molyorbital range which includes benzene (shown later) to show both localised and delocalised p orbitals to represent the hybrid pi-orbitals; hybrid sigma orbitals are also shown. One Minit model is shown using the flexible double bonds, a feature also offered for the Orbit and Molymod sytems. This method is not ideal for some molecules, e.g. aromatic rings because of the distortions introduced when using an sp^3 atom centre rather than the correct sp^2, see Concluding Thoughts.

Summaries of features for the five brands covered with a kit from each range

Note on local availability. The kits will be most readily available in their country of origin. Some maker's have local distributors outside place of manufacture. If not available locally, some maker's websites or third parties do offer shipping abroad, but from the author's experiences of importing US kits to the UK, the shipping and import costs are high relative to kit cost, so overall cost needs to be evaluated.

Brand: ChemKits, Inc. Country of origin: Made in the USA. **Parent website:** chemkits.com

Atoms: Pre-formed coloured metal alloy atom centres called 'valence clusters' - tetrahedron (sp^3), trigonal bipyramid (sp^2), octahedron (sp).
Bonds: Bi-coloured plastic tubing for C-H, O-H, C-N plus single coloured tubing.
Bond scale: 1 Å = 1 inch
Notes: In-line connectors for bonds between dissimilar atoms and right-angled connectors to build pi-bonding. Spare parts available online.
Extent of kit range: 'Student', 'Instructor' and 'Classroom' sets in style illustrated. 'General Chemistry' as well as 'Organic Chemistry' sets. Other model types offered e.g. 'Bio Molecules' which include 'MicroMolecules' of relevance in biology e.g. amino acids.
Instructions provided: Brief guide on card in lid. Downloadable 24 page 'Instruction Manual Framework Molecular Models from the earlier 'FMM' kits (available on the maker's website). The manual is well illustrated and straightforward to follow providing a range of example molecules to build.

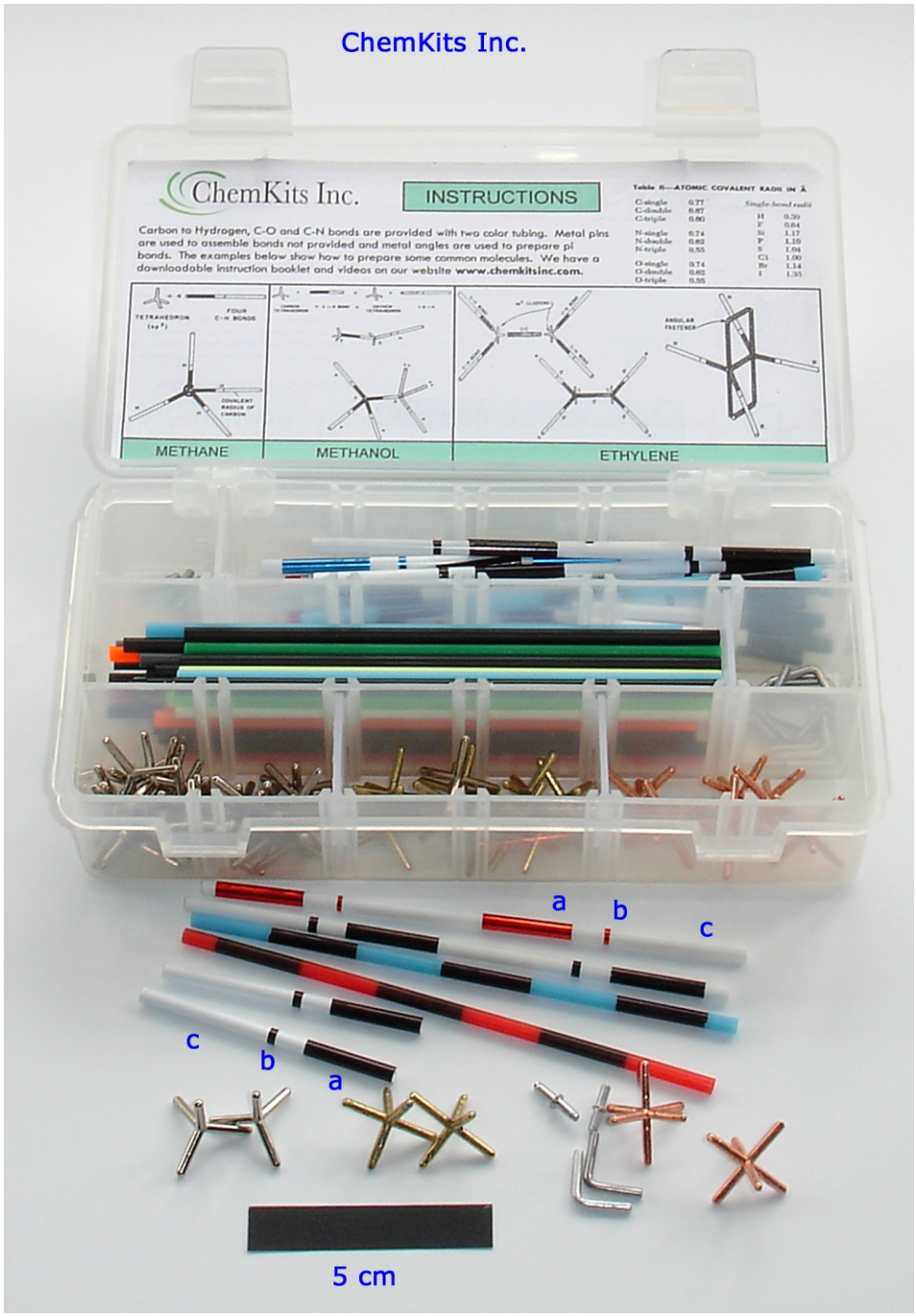
Comments: Bonds in kit bought in 2016 require the plastic tubing to be cut by a user with a sharp knife e.g. safety razor blade advised. Supervision of younger users may be needed. ChemKits usefully notes that, 1) the bi-colour tubing of current kits has a harder wearing finish than the original FMM kit, 2) the kit shown has uncut bonds but these are being replaced with both precut bonds and tubing for user to cut their own.

Typical kit: 'Organic Chemistry', price within US $39.99 (Mar 2017). *Price includes free delivery in the contiguous United States. Illustration next page.*
Housed in an attractively presented sturdy, compact, compartmentalised box, it keeps items separate and ready for use. The preformed metal alloy atom centres are shown; tetrahedral, bipyramidal and octahedral. The bi-coloured tubes represent common two atom bonds (3 per tube) which are cut off. Solid colours for own bonds are also included.

This kit for C-H, O-H and N-H has preformed bonds (2 per tube) showing for e.g. C-H, the C and H covalent radii (a), the position of the H nuclei (b) and extended tubing (c) to show the van der Waals radii of the hydrogen. This feature can prove valuable especially when studying e.g. intramolecular steric hindrance, conformational analysis etc.

The in-line metal connectors allow the user's own bi-atomic bonds to be built and the angled connectors allow pi-bonds to be illustrated (delocalised in the case of aromatic rings, e.g. benzene as shown in earlier image above).

As the maker's website notes, this kit is based on an updated form of the Framework Molecular Model (FMM) kit designed by Dr George Brumlik in 1965. This was the kit sold under the Prentice-Hall brand recommended in my mid-70s UK college chemistry course and still own it, shown above. These older kits can sometimes be found sold used e.g. on auction sites. The paint for O-H, C-H and N-H was prone to wear on these older kits.



ChemKits Inc. 'Organic Chemistry'.

Brand: Minit from Cochranes of Oxford Ltd. Country of origin: Made in the UK. **Parent website:** www.cochranes.co.uk
The website notes that they are family run business since 1962.

Atoms: Coloured pre-formed plastic atom centres 0.6 cm diameter. Including tetrahedron (sp^3), trigonal bipyramid (sp^2), octahedron (sp). See Notes on bond angles. Lattice set includes 8, 12 coordination centre atoms.
Bonds: Precut plastic tubing for common bond lengths plus uncut tubing. Includes flexible tubing for double bonds.
Bond scale: 1 Å = 2 cm (deduct 0.6 cm off bond lengths for the two atom centre radii).
Notes: Both the Minit and Orbit sets have three coded non-linear diunivalent and four trivalent atom centres with different bond angles. The Minit atoms have bars marked to indicate the variants; the trivalent atoms supplied are used e.g. in strained rings or peptides.
Spare parts available online.
Extent of kit range: 'Student' and 'Group' sets offered. Three kits in same presentation style - 'Organic and Inorganic chemistry', 'Modelling Biochemistry', 'Modelling Lattices'.
Instructions provided: Themed booklets included with appropriate Orbit / Minit kit and cover both set types. Author R S Lowrie. Well written and extensively illustrated with molecules to build.
'Organic and inorganic chemistry' 50 pages, pub. 2005. 'Modelling Biochemistry' 46 pages, pub. 2004. 'Modelling Lattices' 37 pages, pub. 1973.
These booklets are excellent and include tables of bond lengths to use either the closest pre-cut bonds or the size required to cut for greater accuracy. The atom centres are deducted off the bond tubing lengths.

Typical kit: 'Organic and Inorganic Chemistry Student Set 0073'. *Illustration next page.*
UK price £23.85 (Mar. 2017, Amazon UK).

A simply presented kit in a non-compartmentalised container. Similarly styled sets are available for 'Modelling Biochemistry' and for 'Modelling Lattices' each supplied with its own booklet (the other two booklets can be bought separately and are shown but not included with the set shown). Contents overlap to some extent for the three but the atom distribution reflects the main studies that each set is intended for.

Coloured atom centres (6 mm diameter) are included for various coordinations as shown. Precut green and red bonds are included and uncut to cut own bonds more accurately. Flexible white tubing is supplied to cut double bonds and hydrogen bonds.

This is the kit which builds the smallest molecules of the five discussed, which can have both pros and cons.

Pros: With 320 atom centres it is arguably the best value for those on a budget, especially if wanting to build complex molecules without the need for more kits / parts and if wish to keep molecules compact. The small molecules are best suited for personal / small group study as rather small for demonstration purposes.

Cons: For an adult I found it the fiddliest kit to use, the plastic pieces are slippery and not that easy to press the tiny univalent centres for example into the tubing, this may improve with repeated use. The tubing is less flexible than for the Orbit and some links can become loose quite readily which may affect the rigidity of larger molecules.
Keeping track of the variants of the two and three pronged centres for the small pieces may be better suited for individuals building with care rather than in a group. Although for non-critical models the differences of bond angles can be overlooked.

(I use small bags for each of the Minit atom centres to keep track of them, especially useful for the different trivalent atom centres).

Minit from Cochranes of Oxford 'Organic and Inorganic Chemistry Student Set 0073'.

Brand: Orbit from Cochranes of Oxford Ltd. Country of origin: Made in the UK. **Parent website:** www.cochranes.co.uk
The website notes that they are family run business since 1962.

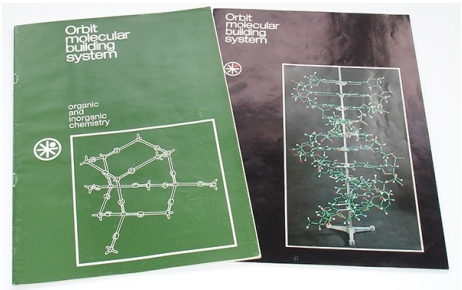
Atoms: Coloured pre-formed plastic atom centres 1 cm diameter. Including tetrahedron (sp^3), trigonal bipyramid (sp^2), octahedron (sp). See Notes on bond angles.
Bonds: Precut plastic tubing for common bond lengths plus uncut tubing. Includes flexible tubing for double bonds.
Bond scale: 1 Å = 3 cm (deduct 1 cm off bond lengths for the two atom centre radii).
Notes: Both the Minit and Orbit sets have coded non-linear diunivalent and trivalent atom centres with different bond angles. The Orbit atoms have the degrees marked to indicate the variants; the trivalent atoms supplied are used e.g. in strained rings or peptides. Spare parts available online.
Extent of kit range: 'Individual' and 'Class' sets offered.
Instructions provided: Themed booklets included with appropriate Orbit / Minit kit and cover both set types. Author R S Lowrie. 'Organic and inorganic chemistry' 50 pages, pub. 2005. 'Modelling Biochemistry' 46 pages, pub. 2004. 'Modelling Lattices' 37 pages, pub. 1973.
These booklets are excellent and include tables of bond lengths to use either the closest pre-cut bonds or the size required to cut for greater accuracy. The atom centres are deducted off the bond tubing lengths.

Typical kit: 'Organic and Inorganic Chemistry Class Set 0047'. *Illustration next page.*
UK price £48.37 (Mar. 2017, Amazon UK).

The Orbit sets are a well established British kit and I used a comparable version in the mid 70s. The principle is very much the same as the Minit, also from Cochranes, except that the atom centres are 10 mm not 6 mm. For an adult the larger atoms are easier to handle during assembly. The 3 cm rather than 2 cm scale for 1 Å for the Minit gives larger molecules both for individual inspection and demonstration. The compartmentalised box also keeps the piece types separate

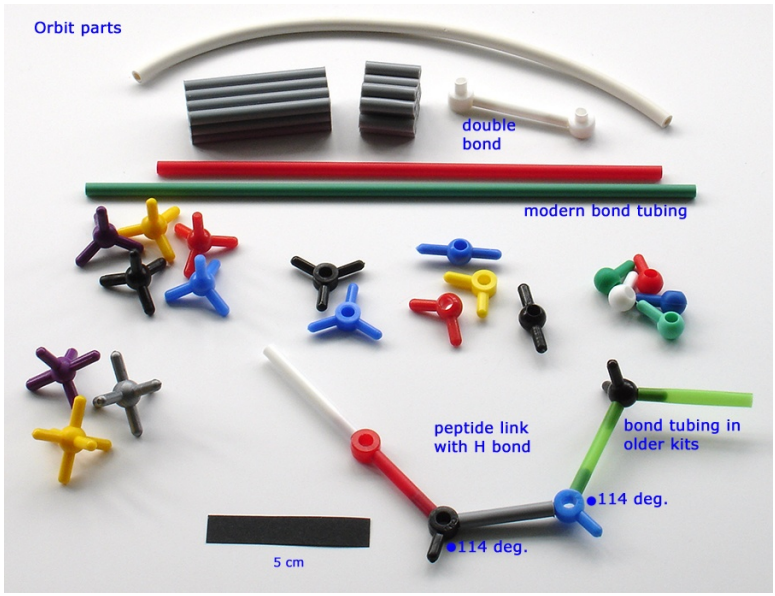
In the modern sets, shown on the next page and as for the Minit, pre-cut bonds close to typical common bond lengths are now supplied and aids quick assembly. The tubing also has a more rubbery texture than the brittler bonds in older kits making for more secure links. Longer tubes are also provided to cut own including flexible tubing for e.g. double bonds (a few are shown built in the box) or strained rings.

Buying used: Older Orbit kits can often be found used in the UK and can be good value if on a budget. The author's original mid 70s Organic / Inorganic kit is shown below and a Biochemistry kit from the same era, the latter which was recently offered unused in the Oxfam online shop for a fraction of a comparable kit's new cost. The Biochemistry kit could build the part DNA helix shown on the box. Pre-cut bonds were not offered. The manuals provided more advanced guidance than modern sets e.g. on building a protein alpha helix as was the only accessible approach for many users at the time for quantitative studies.



Orbit 1970s kits for Organic Chemistry, Biochemistry and the manuals.

'Organic and Inorganic Chemistry Class Set 0047'.
Below, parts include one of the dedicated trigonal atom centres for special cases, e.g. 114° for peptide bonds



Brand: Molymod Country of origin: UK. **Parent website:** www.molymod.com
The website notes that Spiring Enterprises Ltd are the inventors and sole manufacturers of the Molymod range.
Thank you to Molymod who note that the kits 'are widely available around the world through local distributors'.
Atoms: Coloured plastic spheres 17 to 23 mm diameter with ports of various coordination for bonds.

Hydrogen: Compact and open models: 17 mm 1-hole.
Compact 'semi-space-filling' only: "mushroom'-style Atom links'.
Two sets also have 'half-sphere Molydome' 19 mm.
Bonds: single bonds are 19 mm 'medium links', multiple bonds are 30 mm 'flexible links', compact models have 2 mm 'short links'.
Bond scale: Open / ball and stick 1 Å = 2.5 cm, closed / semi-space filling 1 Å = 1.5 cm
Notes: Kits with short 2 mm links have special link removal tool included.
Extent of kit range: 'Student' and 'Teacher' sets for many kits. Kits include 'Organic', 'Inorganic / Organic', 'Biochemistry', 'Advanced Level Chemistry'.
Special kits include: inorganic lattices e.g. diamond, graphite, sodium chloride; organic space filling e.g. peptides (alpha helix, beta pleated sheet, chains,), fat (glyceryl tristearate), sucrose, glucose, starch.
'Molyorbital' sets to show the shapes of various bonding orbitals and for specific molecules such as benzene and simple inorganics.
Instructions provided: Typically a two page leaflet describing the parts and their use in construction illustrated with typical molecules. Leaflet illustrating the kit range included.

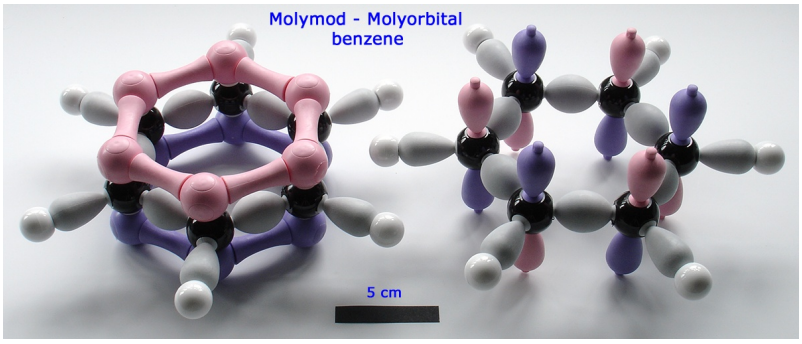
Typical kit: 'Inorganic / Organic Teacher Set MMS-004'. *Illustration next page.*
UK price. £35.65 (Mar. 2017, Amazon UK). *Molymod notes that the kits are widely available through local distributors outside of the UK.*

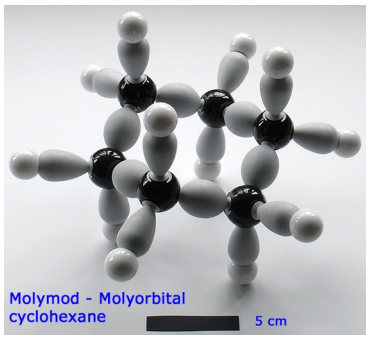
The long established Molymod sets are British designed and made by Spiring Enterprises Ltd. They offer a 'dual scale system' for building models—either an 'open' ball and stick style or 'semi-space-filling'. The grey / purple links shown are used for the former, the short white links for the latter. Pressing the links fully home into the atom centre holes and later removal can require quite a firm action especially when new. The tool shown works well to remove the short links.

A wide range of kits are offered and typically housed in one or two sturdy plastic boxes; some are compartmentalised with stackable trays, e.g. the 'Biochemistry Set'. The one shown has the parts supplied in bags. These bags can be usefully replaced as here with resealable varieties to keep the parts discrete if wished.

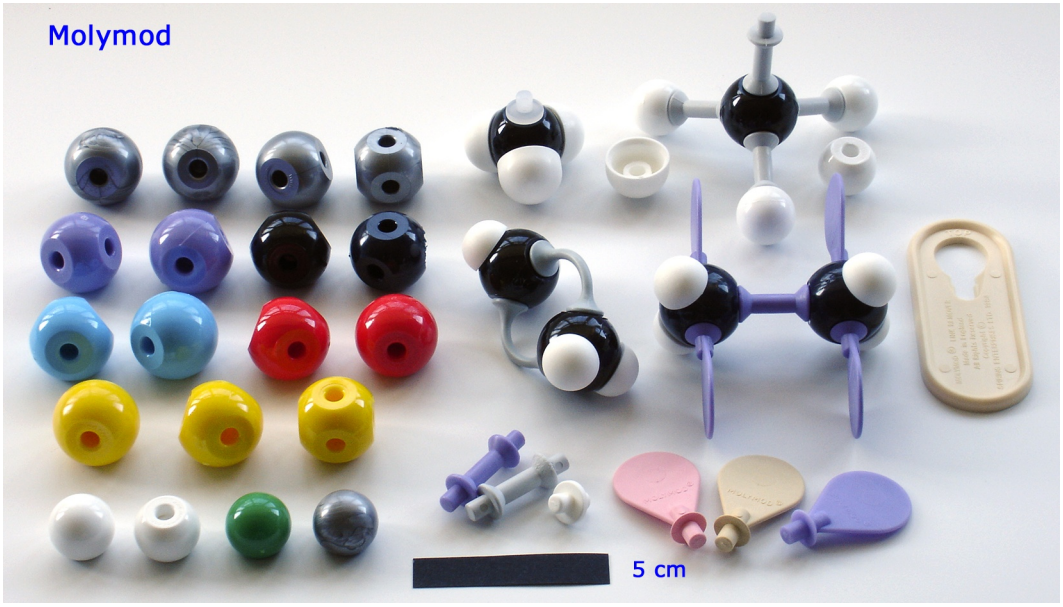
Atom parts where appropriate are supplied in a range of coordination centres. Depending on the kit, hydrogen atoms are supplied as spheres, Molydomes and/or 'mushroom-style' (see methane and ethene depictions on next page). The latter form are recommended for constructing 'semi-space-filling' models. Double bonds in ball and stick models can be shown using single links or two flexible bonds as shown for ethene. The purple links can be used to highlight aspects of certain bonding types e.g. hydrogen bonds— I often use them for double bonds. If using the flexible links for double bonds, tetrahedral carbon centres are used. The 'pear shaped lobes' supplied can depict localised p orbitals if desired in unsaturated molecules or lone pairs of electrons on atom centres.

Molymod also offers a special Molyorbital range (not part of the MMS-004 kit illustrated) which includes benzene (left below) to show both delocalised and localised p orbitals, the former to represent the hybrid pi-orbitals. The sigma orbitals (in grey) are also shown in these benzene models and also in the model of cyclohexane (right below).





Upper left Molymod.'Inorganic / Organic Teacher Set MMS-004'. I've replaced the bags with resealable ones.
Upper right:'Biochemistry Set MMS-007'. Double boxed, with two layers of trays. This set was used to build the alpha helix.
Lower left. 'Organic Teacher Set MMS-003'. Lower right. 'Semi-space-filling set for Organic Chemistry MMS-005 v2'.



Molymod atom centres, bond links, hydrogen forms (illustrated with part assembled methane), double bond options (ethene), electron lobes and link removal tool. The distribution of parts varies between the kits. Not shown are CII and CIII centres offered in the organic sets and also some other centres such as additional halogens. CII are used e.g. for carbon atoms with triple bonding. Some sets also offer flexible 'V-links' for constrained rings.

Brand: Molecular Visions (Darling Models, Inc.) Country of origin: USA.
Parent website: www.darlingmodels.com (buyers within USA) www.molecularvisions.com (non-USA buyers)

Atoms: Coloured atom pieces to construct atomic centres of various coordinations, including tetrahedral, trigonal bipyramidal, octahedral.
Bonds: Preformed bonding pieces used in conjunction with atomic pieces to create e.g. pi-bonds.
Bond scale: 1 Å = 2 inches
Extent of kit range: Kits suitable for individuals and 'Instructor Demonstrator' kits offered. Biochemistry. Additional specialist components e.g. cylopentadienyl ligands. Extensive range of kits using same system to build specific structure s e.g. fullerenes, ice, protein alpha helix, amino acid base pairs.
'Solid State General Chemistry' kits offered using a different versatile system.
Instructions provided: Leaflet illustrating assembly methods.
'A Guide to Framework Molecular Modelling' by Stephen D Darling, 48 pages in colour. Pub. 2001. Can also be downloaded.
Kits for solid state models have available the 40 page 'Solid-State General-Chemistry Molecular Visions Models' by Stephen D Darling. Pub. 2005. Can be downloaded off maker's website.

Typical kit: #1 Organic, Inorganic, Organometallic
Price within USA on www.darlingmodels.com $25 including shipping (Mar. 2017)

Parts are supplied in a custom fitted box. The other four kits discussed use pre-formed coordination centres for each atom. The Molecular Visions system uses part formed atom centres / bonds as illustrated below which click together using a proprietary 'push/pull coupling system'. This may not be as immediately intuitive as other model kit systems, but once familiarity is gained, possibly with supervision for students, it is a very powerful and versatile system.

The typical kit illustrated also supplies a limited number of 'marker balls' for highlighting key atoms that do not form part of the main skeletal framework. As remarked above, this can have benefits for clarity rather than showing all atoms in the molecule. This approach can also be adopted with other kits if desired.

Typical Molecular visions parts. Additional parts are available. The system builds atom centres using a 'push / pull coupling system'.

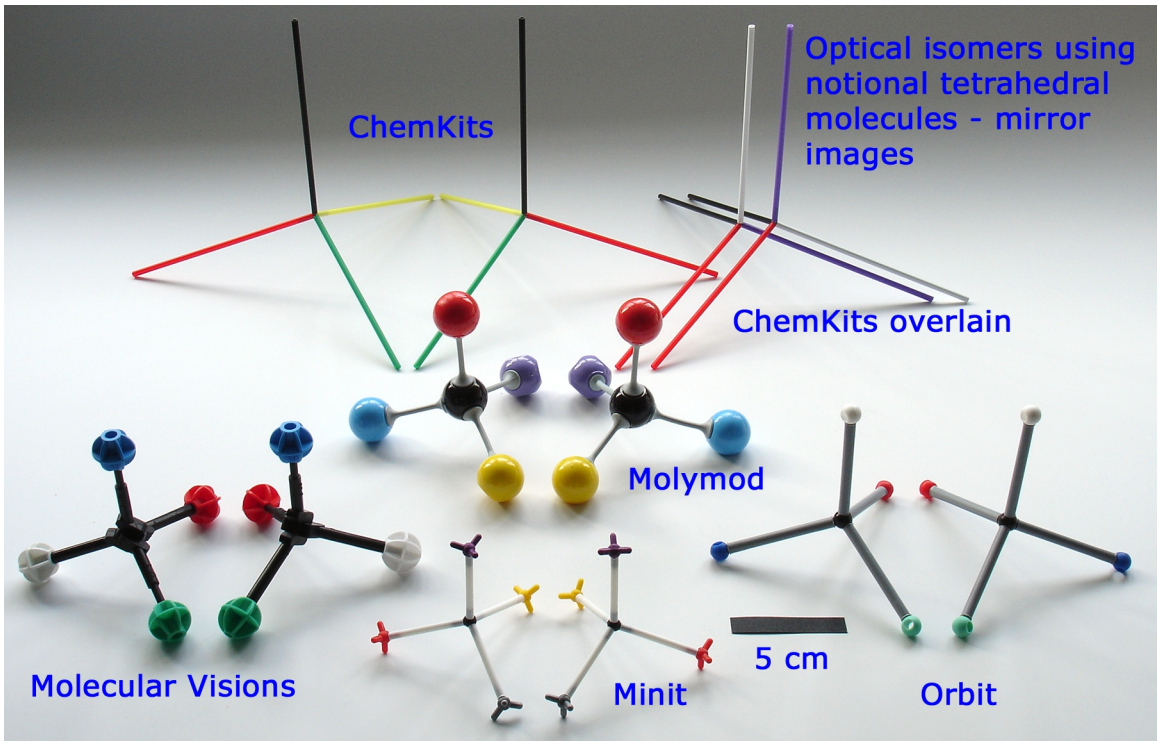
#1 Organic, Inorganic, Organometallic
Price within USA $36.75 (Nov. 2016)

Optical isomers - the asymmetric (chiral) tetrahedral carbon

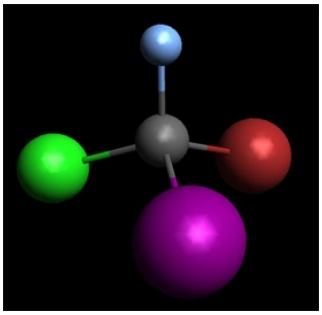
Demonstrating the concept of optical isomers is perhaps one of the simplest but arguably one of the most effective uses of physical kits rather than software. The mirror images of chiral carbon atoms in *notional* molecules are shown for all the kits in the image below (with the true CPK atom colours being ignored in these cases). The ChemKits molecule can just make use of the full length coloured bonds supplied which are also ideally suited to show that isomers do not match if overlain. For group demonstrations, the kits with larger atom centres or coloured bonds may work best, less so for the Orbit and Minit kits.

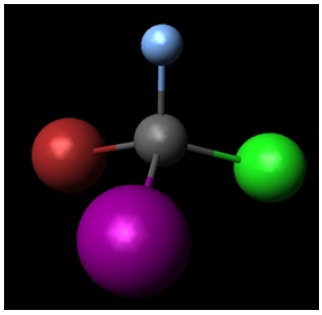
Are kits more fun than software? In a group, each student could be supplied with a tetrahedral carbon atom and four coloured atoms / bonds and asked to build a molecule. There will likely be a mix of the two isomers made and could ask neighbouring students to try overlaying their molecules to add a fun aspect to the study of optical isomers. The use of physical models also helps aid a user's understanding of, for example, the different conventions used for representing molecular structures in print.

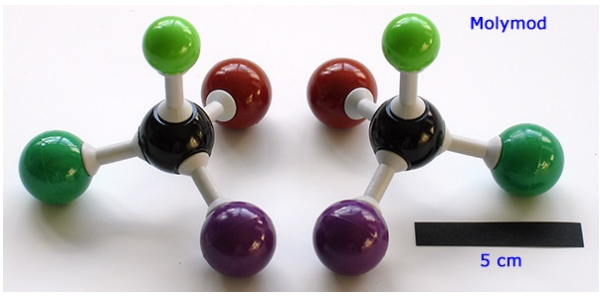
Below. Representation of optical isomers of a chiral tetrahedral carbon centre using the five kits. Showing the mirror image symmetry.



Software note: *Building single carbon chiral molecules is easy with a kit and takes very little time. Users familiar with software would also likely accomplish this task quickly but beginners may need guidance.*

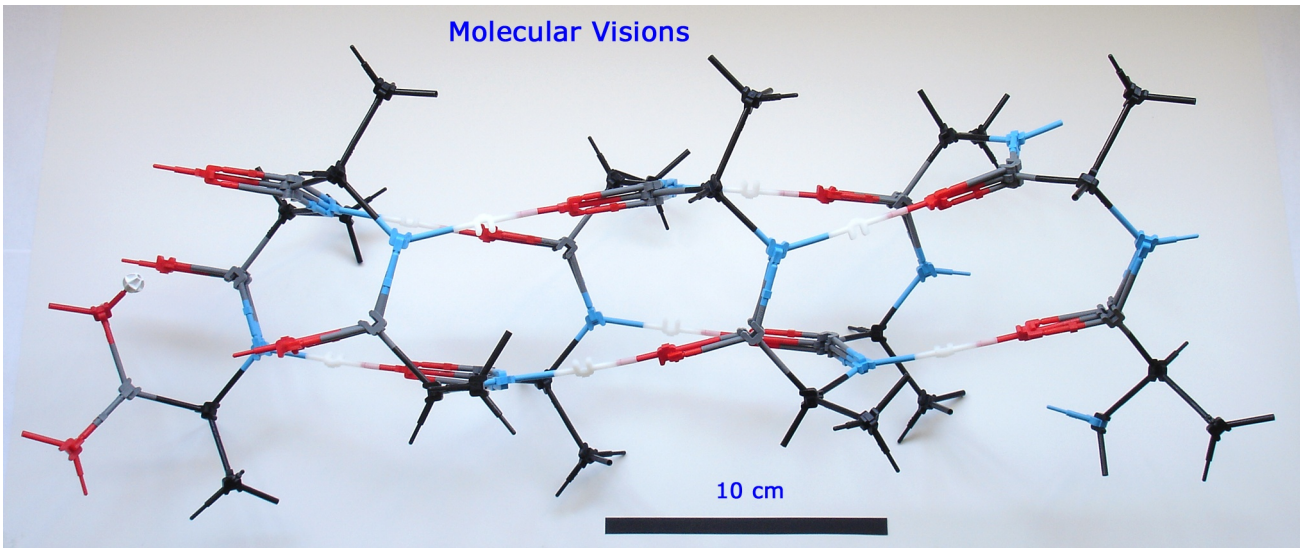




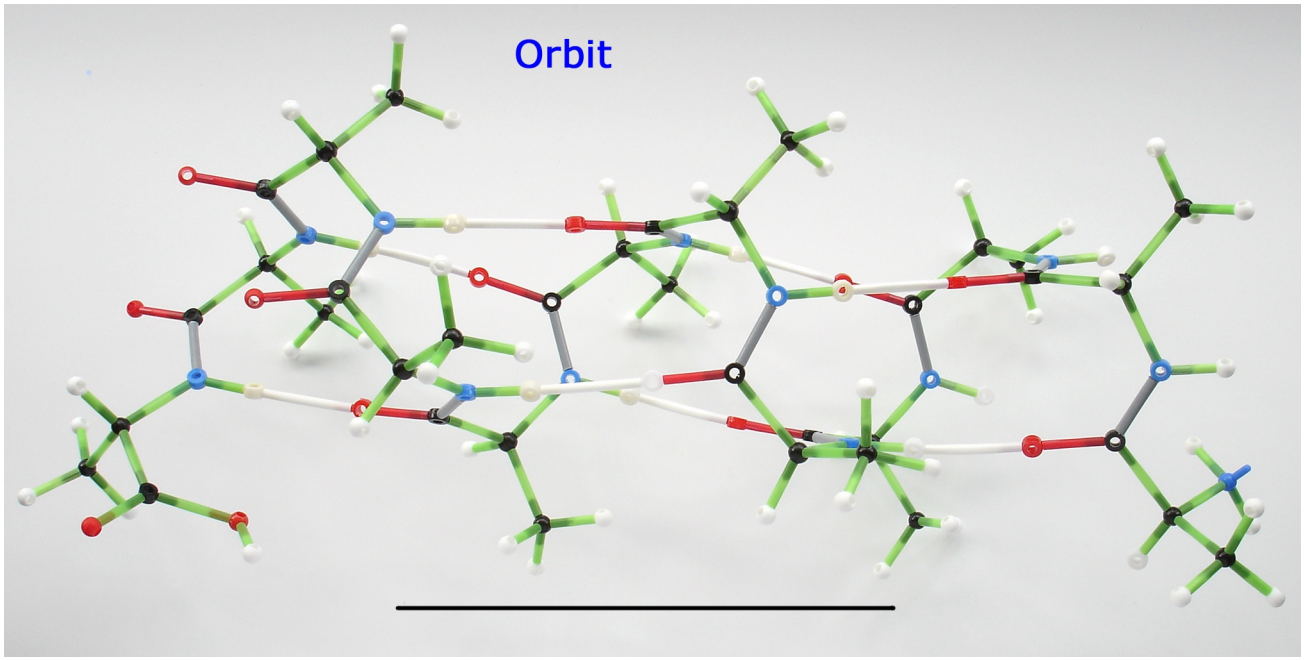


Above (left and middle). A molecule with a chiral carbon atom created in Avogadro software and its mirror image. Despite spending some time learning Avogadro, (I'm on a learning curve myself), this simple task of creating a mirror image seemed non-intuitive compared with physical model building, not helped by Avogadro crashing with a simple copy command. So the images above were created by making one isomer in Avogadro and using a feature in Photoshop for the mirror image. If not using physical models, step by step interactive lessons on screen may work better to show some concepts e.g. see the University of Illinois demonstration.
Above right. The Molymod open model equivalent for comparison of CFClBrI.

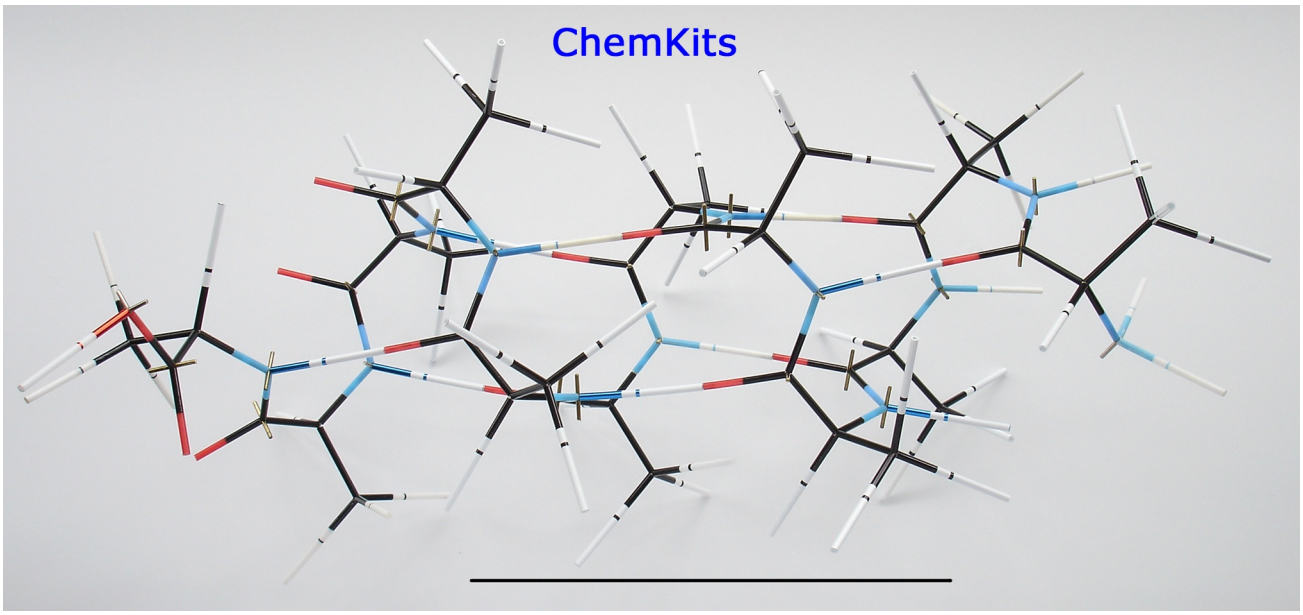
Comparison of kits for building a more complex molecule - part of a protein e.g. L-alanine alpha helix
The right handed spiral of L-alanine is commonly used to illustrate one of the types of secondary structure, the alpha helix, that proteins may adopt. The scale bar shown for all is 10 cm which illustrates how the sizes vary for comparable lengths of helix. Building a larger molecule is useful to compare and contrast the relative merits of the kits for this purpose. Robustness in handling becomes more important, especially if handled by groups. The Molecular Visions and Molymod were the best in this regard. For the other three kits used, some looser fitting bonds can occur but can be spotted during construction and replaced, the Minit and older Orbit systems seemed the most prone.



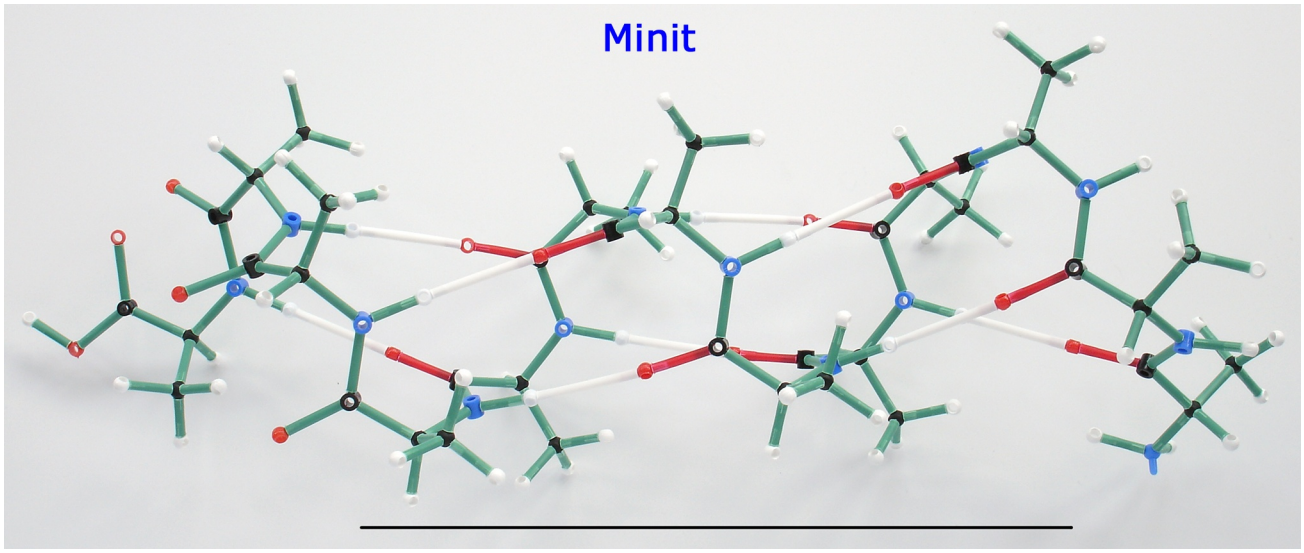
Above. Molecular Visions, using their dedicated kit #9 'Protein alpha helix' ($16-50) with methyl groups. The kit includes leaflets showing the full structure and construction notes. Note the 10 cm scale bar, this model is much larger than the other four. A particular merit of this design of kit for large molecules is the structural rigidity and large size i.e. especially suited for heavy handling in an educational group setting. The peptide groups stay planar, a key aspect of understanding the structure of polypeptides. The white bond links are the hydrogen bonding that is responsible for the secondary structure. Construction using this system is more involved than for the other four, the C=O with H bond is a three piece structure and a little awkward to make.



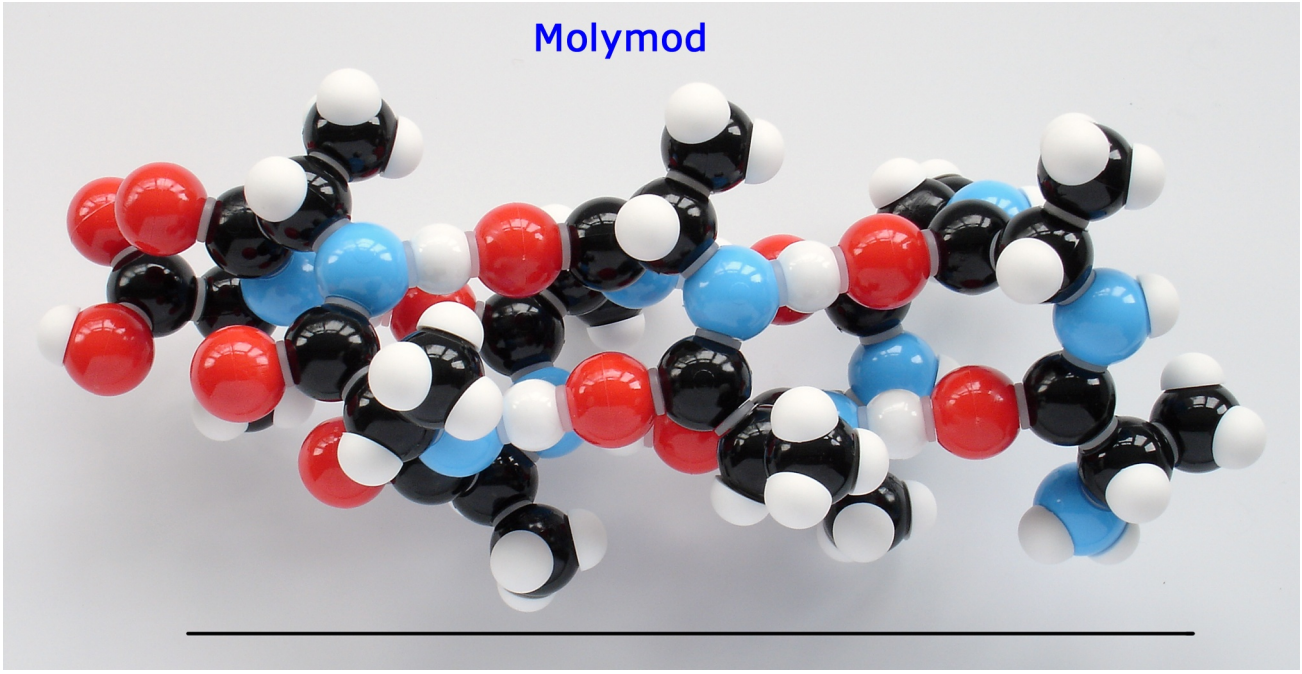
Above. Orbit. For this construction I used the correct trivalent C and N atoms for the peptide groups with the correct bond angles supplied and cut bond lengths. The coloured bond links supplied can be used to highlight the different types, in this case grey for C-N, red for C-O, white for H bonds*. Peptide groups CO.NH are planar because of electron delocalisation and the C and N atoms in each peptide deviate somewhat from 120º. Trivalent C and N centres with 114º angles are supplied. The bonds are also intermediate between single and double bonds. Keeping track of these near identical atom centres to standard 120º trivalent centres during construction and disassembly can be awkward, especially if a group study. See note below on accuracy in building molecules with kits. (*As I already had precut accurate green bonds from my 70s kit, these were used. Modern kits have a darker green more rubbery tubing. See Minit model below.)



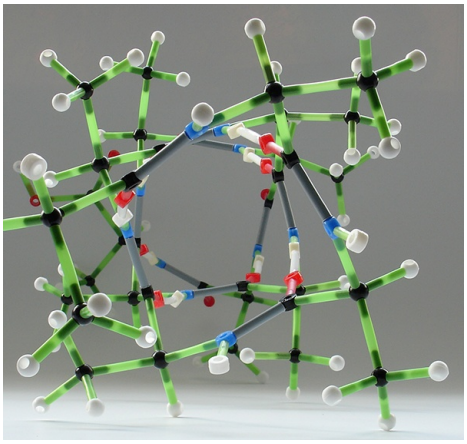
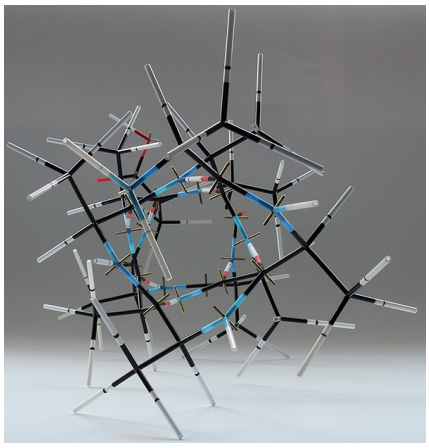
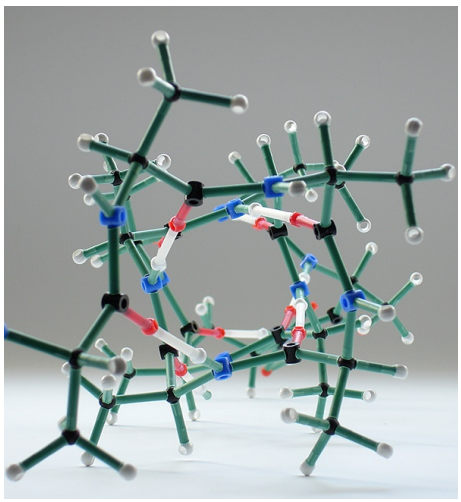
Above. ChemKits. My old and new examples of this kit were used to construct the molecule. Showing the van der Waals distances of the O-H, C-H and N-H bonds are a feature of this kit. Molecular structures can have an aesthetic appeal as well as educational and find the skeletal form of the polypeptide very elegant with use of coloured bonds showing the core black helix well.



Above. Minit. As for the Orbit kit the correct trivalent atom centres for the peptide C and N atoms were used. The pre-cut bond lengths supplied were used throughout which approximate to many bond lengths. This budget kit is arguably the most cost effective to build more complex molecules. The scale used also gives compact molecules suited for individual study. The small coloured atom centres don't stand out well against the bonds and not as clear as for example the ChemKits to show the core of the C-N helix.



Above. Molymod. This was constructed using the system's 'semi-space-filling' method offered. The medium links can be used to make a ball and stick model. The more comprehensive 'Biochemistry Teacher's Set' MMS-007 that I own was used for this construction not the MMS-004 illustrated earlier; the former includes the short links and mushroom hydrogens. This type of model more closely approaches what the true molecule looks like. The ball and stick and skeletal models can be the more useful for showing interatomic relationships. In this regard, models of different types can be complementary to show these different aspects. As for the ChemKits, I also find these type of models aesthetically very pleasing and tactile.

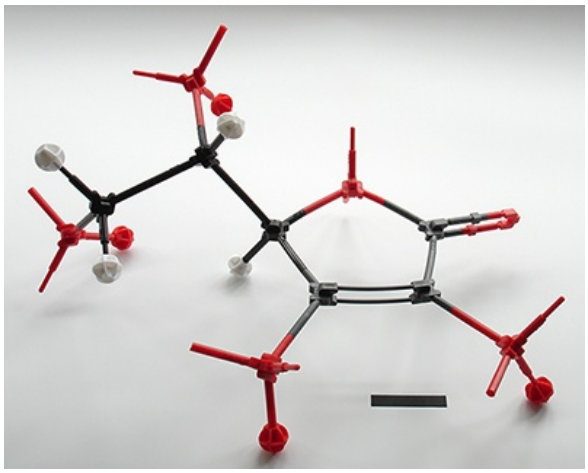

Above. End views of the Orbit, ChemKits, Minit and Molymod alpha helix. The first three are the more successful at showing the helical pattern from this perspective. The Molecular Visions not shown but also shows well the helix.

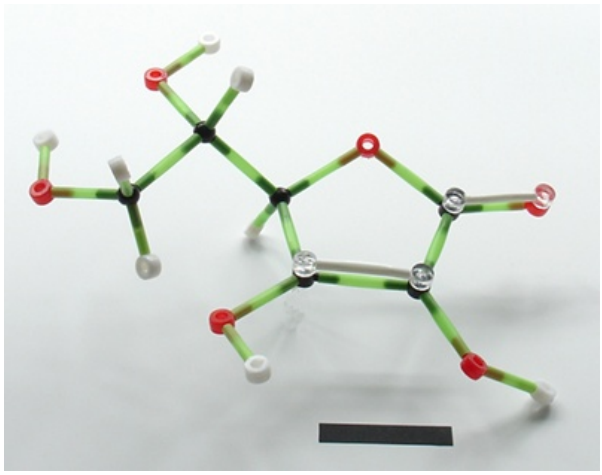
Software note: *Relative merits of using either software or a kit to build increasingly complex molecules such as the above alpha helix.*

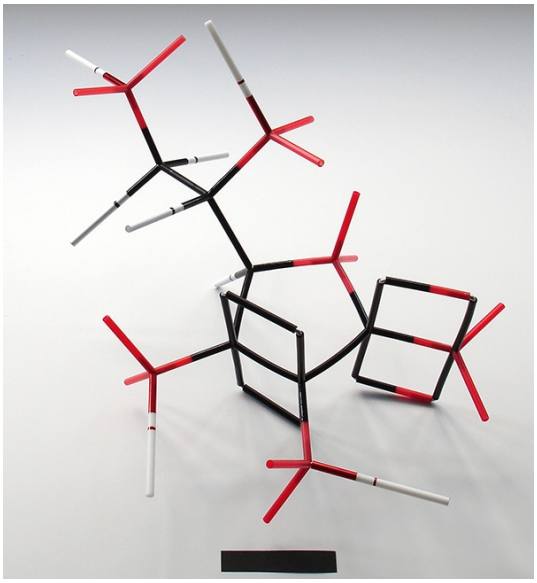
Software:
- As a molecule becomes more complex, rather than building from atoms, it is common to download pre-built molecules from various databases if a source known. (I struggled to find the alpha helix shown above from databases as there are so many variants.) To build a molecule which has secondary structure from scratch will require good familiarity with the software.
- Allows rapid interchange between various molecular structure representations such as skeletal (wireframe), space-filling, depicting all van der Waals radii / surfaces etc.
- Offers sophisticated features both qualitative and quantitative that a physical model can't easily replicate with accuracy.

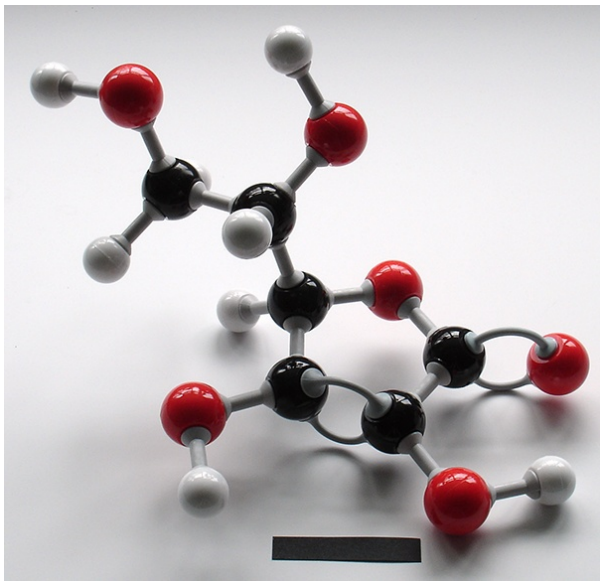
Model kit:
- Building this type of molecule as a kit can be very satisfying, especially in an educational setting. As add more peptide groups it becomes clear how the hydrogen bonding acts and which is key to forming the helix. A number of makers offer cost effective dedicated kits for such models so only need to buy the parts required.
- Arguably, more could be learnt by building such a physical molecule, either as an individual or as a group in an educational setting, rather than downloading a pre-built molecule with no participation in its construction and just viewing at various angles on screen. Group activities could involve, for example, small groups building peptide links to assemble together as an alpha helix or other structures such as the beta pleated sheets.

Vitamin C (L-ascorbic acid) This molecule illustrates how localised double bonds (C=C and C=O), electron lone pairs and O-H, C-H bonds can be represented in the different systems. Some systems offer alternative methods.







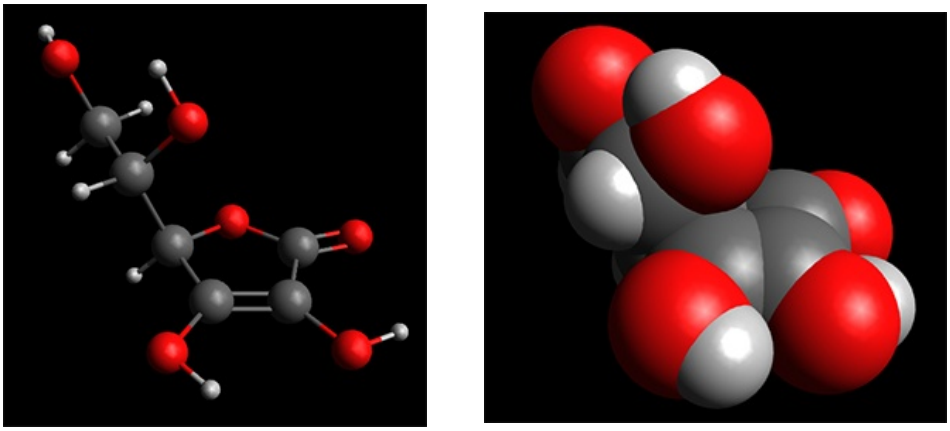


(5 cm scale bar)

Molecular Visions (top left) - In this system the marker atoms supplied can be used as desired. Here white atom markers show H attached to C and red attached to O. Electron lone pairs are shown using tetrahedral O centres. Marker atoms supplied as standard (up to six per atom colour) are limited but can be bought as spares.
Orbit (top right) (Minit is comparable at smaller scale) – double bonds are shown as white bonds. An option is provided to show double bonds show with flexible links and tetrahedral atom centres (e.g. see Minit benzene above).
ChemKits (bottom left) – the pi orbitals of the double bonds are shown at the correct van der Waals distance. Also for the O-H and C-H bonds. This system can be useful for exploring intramolecular steric effects of suitable molecules with a physical model. Each oxygen's two electron lone pairs are shown on tetrahedral atom centres as red bond links
Molymod (bottom right) – the molecule was built using the 'medium' length links to show the 'open' ball and stick form. Double bonds shown using flexible links and the tetrahedral centres. They could also be shown and highlighted with the purple single links and the sp^2 carbon centres with optional pi-electron lobes supplied. Oxygens in O-H are shown with the two coordinate atoms so lone pairs not shown. A tetrahedral centre could be used for these oxygens plus the electron lobes shown (see benzene above)

Software note: The potential complementary roles of physical models and the use of software. The vitamin C models above provide a simple example. When photographing the Molecular Visions and Orbit models, the optimal geometry was not considered and may not be too clear what it may be with multiple lone pairs and nearby hydrogen atoms.

Building the molecule in software or downloading the file from a database allows the geometry to be optimised. The ChemKits and Molymod photos are shown above with calculated optimal geometry using Avogadro software (below), i.e. with carbon atoms in side chain planar and O-H orientation as shown. The software model is also shown right below with all van der Waals distances. Software allows a one button click to flip between forms. This form is particularly valuable for studying some aspects of intermolecular interactions and haven't come across to date modern physical kits that show this form. For many intramolecular studies this form is of more limited use.



Above, Vitamin C with calculated optimised geometry as depicted in Avogadro software. Left ball and stick, right – van der Waals distances show the true structure on the molecular scale. Both same scale.

Note on accuracy when building kits

Two approaches are possible when building a molecule—where offered, to cut accurate bond lengths appropriate to each kit's scale or use of the nearest pre-cut bond lengths. Some of the kits allow both options; Orbit and Minit also offer the special trivalent atom centres found in molecules such as those with peptide links. Each user needs to balance convenience and accuracy. In many circumstances the need for accuracy has changed for physical molecules since these kits were first offered in the 60s - 70s. At that time there was no software readily available to most users. (Students like myself learnt computing by typing out programs on punched cards for an unseen mainframe running Fortran.) The Orbit manuals I possess from the 70s kits placed more emphasis on accuracy in e.g. polypetide construction as that was the only accessible approach for accurate studies for a student.

Nowadays, everyone has access to software packages, many free, that can build / visualise molecules from the simple to the complex. They can be built from scratch or download ready made models in various file formats from online databases. Such software once familiar with it, offers a wealth of sophisticated features for quantitative studies such as bond lengths, bond angles, van der Waals distances etc.

The homebrew box right of own cut bonds for the Orbit kit from the 70s but many bonds only differ by a few mm each at the standard scale used and not entirely necessary.

Concluding thoughts. All the kits work well, are great fun, educational to use and offer different approaches and scale to present molecules. Many molecular models also have a pleasing tactile and aesthetic appeal. As remarked, an individual or group choice of brand may be largely governed by local availability if no particular kit is recommended in an educational setting. Different styles of kit can be complementary depending on what aspects of a molecule a user wishes to show. Some are also more suited to build larger molecules, depending on scale and budget.

As the Vitamin C example shows, it doesn't need to be either / or for physical kits / software, they can also be complementary and no doubt are for many users. One of the valuable complementary roles of software in education is the ability to flip between or mix representational forms such as skeletal, ball and stick, van der Waals surfaces etc. Arguably, most quantitative studies would be more readily carried out nowadays in software. Larger scales chosen by the user can be adopted with physical kits that use variable bond lengths for more accurate quantitative studies

However, in some roles, despite beautiful rendering on screen offered by most software, a representation can't match handling a real 3D model if possible. There can be a steep learning curve with software and without guidance have the potential to mislead, e.g. the cyclohexane example. For many educational scenarios it can be argued a physical model is the superior for demonstrating concepts e.g. conformers and stereoisomers. Some institutions also build large physical models of macromolecules to aid research.

Of course, compromises inevitably have to be made with physical models so can potentially mislead and their limitations also need addressing in an educational arena. They are stylised to help show interatomic structural relationships but are far removed from actual 'space-filling' form unless all van der Waals surfaces are shown (e.g. vitamin C software model, right above). (I'd be interested to learn if there are modern space-filling kits as haven't come across any. Walton devotes a chapter to 'space-filling molecular models' and tabulates eight makers in her book published in 1978, ref. 3. Francoeur, ref. 1a, notes that they were for sale from Fisher Scientific Education division as recently as 1997.)

An optional approach suggested for some kits to show double bonds may also potentially confuse the beginner without guidance i.e. using tetrahedral atoms and two flexible links to form double bonds (using sp^3 centres instead of the correct sp^2); a point noted by Ingham (1988, ref.2).This approach may also become unwieldy e.g. for molecules with extensive double bonding and can also introduce bond angle distortions so not recommended for aromatic systems. The alternative approaches typically offered may be preferred, e.g. to either highlight the double bond using a contrasting coloured single link or to use a parallel (white) bond using the correct coordination centre; the latter better at representing restricted bond rotation. Although Walton notes (1978, ref. 3a) that white bonds ideally should be used both sides of the sigma bond to accurately represent pi-bonding. Some kits, as illustrated, offer features to show localised and/or delocalised bonding. The Molyorbital sets specifically designed to do this and for orbital shapes.

Both physical models and screenshots (unless further manipulation in software) are also snapshots in time of what may be one of a possible number of stable forms and don't show e.g. thermal effects on molecular structure such as bond rotation. Although with physical models, some possible forms do come naturally to hand, such as the easy flip between chair and boat conformers of cyclohexane. A user may also realise in handling a model that aliphatic chains and functional groups such as -OH can rotate, leading to hands-on explorations of factors such as steric effects. As illustrated with Vitamin C, software can complement studies of physical models to calculate stable forms.

If on a budget, used examples of older or current kits are often available at reduced prices. Check e.g. eBay, Amazon Marketplace etc. As a number of resources discuss (online and see ref. 3), be creative! There are plenty of homemade approaches for simpler concepts; coloured Plasticine / cocktail sticks, cotton wool buds / coloured inks, card could all be used to good effect e.g. to illustrate optical isomers of a single chiral carbon centre and simpler molecules (see Walton, 1978, ref. 3).

Image right, mirror image models to demonstrate chiral carbon centres made with cotton bud stalks and Plasticine.

Comments to the author David Walker are welcomed, particularly any inaccuracies on either the kit descriptions or my possibly rusty chemistry!
The author's work background was in chemistry but not in education.

The author kept both the FMM (now ChemKits Inc.) and Orbit kits used during his college studies in the mid 70s. Modern examples of all the example kits above were bought for the main comparative study.
The benzene Molymod models showing electronic orbitals (and some space filling cyclohexane models) and some additional sets for photography were very kindly donated by Philip Spiring of Spiring Enterprises Ltd.

For clarity, registered trademark symbols have been omitted in the main text but are summarised below as stated on each maker's documentation.
ChemKits, Inc.
Molecular Visions™, Darling Models, Inc.
"Molymod® models are made in England by Spiring Enterprises Ltd. Billingshurst Sussex RH14 9EZ." Other trade marks include Molydome™ and Moly-Orbital™.
Orbit™ and Minit™ molecular models are designed and produced by Cochranes of Oxford Ltd.'

Acknowledgements *(Any errors on the descriptions of the brands and kits are the author's.)*
Thank you to Stephen D Darling, President of Darling Models, for useful discussions on the range and for shipping help from the US.

Thank you to Thomas C. Jempty, ChemKits Inc., for useful discussions on the range and for shipping help from the US. He notes that "the business [FMM] was purchased from the son of the inventor in 2010".

Thank you to Philip Spiring, Spiring Enterprises Ltd for the generous donation of some sets including Molyorbitals and providing an insight on aspects of the range. An illustration of an impressive Molymod model of a large macromolecule made by at Huddersfield University, UK was kindly shared. Illustrating the continued value of physical models of large macromolecules.

All software derived images used the Open Source software Avogadro version 1.2.0 with thanks to the developers for making available this excellent software, offering features from the beginner to advanced worker. See:
Marcus D Hanwell, Donald E Curtis, David C Lonie, Tim Vandermeersch, Eva Zurek and Geoffrey R Hutchison; "Avogadro: An advanced semantic chemical editor, visualization, and analysis platform" Journal of Cheminformatics 2012, 4:17. (Open Access paper.)

References / selected resources on physical molecular models.

1) Eric Francoeur, "The Forgotten Tool: The Design and Use of Molecular Models", Social Studies of Science, 1997, vol. 20 (1), 7 – 40. Freely available as a downloadable Acrobat file at http://journals.sagepub.com/doi/abs/10.1177/030631297027001002
A fascinating discussion which includes aspects of the history of physical models, particularly the Stuart, FHT and CPK space-filling designs, the debates of their merits and later the impact of computer modelling and its relative merits.

1a) *ibid,* page 24.

2) Angela N Ingham, "Models in Chemical Education: An Investigation into their Uses", PhD thesis, Dept. of Educational Studies, University of Surrey, December 1988, page 8. Freely available as a downloadable Acrobat file at http://epubs.surrey.ac.uk/771366/1/234561.pdf

3) Anne Walton, "Molecular and Crystal Structure Models", Ellis Horwood Ltd., UK, 1978.
"The book provides a theoretical and practical guide to all users, discussing the whole range of models available for use today." [1978]. Quote from publisher's summary. Kits discussed include Orbit, FMM (now ChemKits), Molymod, Minit and also homemade alternatives. Now a fascinating historical insight into the large range of kits available at a time predating the ready accessibility to modern interactive computer modelling on all computer platforms.

3a) *ibid*, p. 116.

4) Robert M Hanson, "Molecular Origami. Precision Scale Models From Paper", University Science Books, Sausalito, USA, 1995.
Contains 70 templates of molecules which can be scanned and printed to form models from polyhedra, grouped by the shapes they adopt. Includes buckminsterfullerene.

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Micscape Lite is an occasional feature in an issue where contributors can share their other interests.