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Modular 3D-printed Demonstration Scale Organic Chemistry Model Kit 1

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Giant-Size Molecular Model Kit sold by Sigma Aldrich (Z231312)

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Modular 3D-printed Demonstration Scale Organic Chemistry Model Kit 1

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Abstract

The organic chemistry model kit described here is proposed to substantially increase the service life, serviceability with nonproprietary parts, and long-term robustness compared to other large-scale molecular model kits. The dimensions of the current model kit relate in scale to a commercially available kit (Giant-Size Molecular Model Kit sold by Sigma Aldrich (Z231312)) comprised of painted Styrofoam representations of atoms with cardboard/rubber insertion points (attached to the Styrofoam with staples and adhesive) and painted wood cylinder representations of bonds. The present kit comprises build components derived primarily from 3D printing with extruded thermoplastic (polylactic acid (PLA) filament recycled from post-industrial extrusion waste). The waste materials here can, in turn, continue in the 'closed loop' recycling stream or be bioremediated through industrial, anaerobic composting. The PLA component is an environmentally conscious choice over the existing use of solid-core Styrofoam in the commercially available model kit. 3D printing with PLA filament extrusion makes the present kit extensible. Design enhancements with PLA filament include the ability to vary multiple aspects: color and component flexion. The color (including designer representations branded with school colors or insignia or specialized luminescent colors that can emphasize and contrast relative atom/bond positions) and flexion properties of PLA eliminate the need for paint and reduce the need for different materials to represent the various bond types in organic chemistry molecules, as found in the Sigma commercial model kit. This large-scale molecular model kit includes 155 mm shaft representations of σ -bonds connecting 50 mm spheroid representations of carbon atoms and 35 mm spheroid representations of hydrogen atoms. This kit includes atom representations coupled to at least one 155 mm cylindrical shaft that attaches to an outwardly extending push-to-connect fastener component attached to the surface of the sphere. The assembly of these components illustrates representations of alkane molecules used in organic chemistry to demonstrate the rotational dynamics and perspective representations of acyclic and cyclic alkanes and stereoisomers.

Target Sector

The kit is intended to target students and instructors in the High Schools and University sectors for demonstrations to a live audience in high school, large-attendance university classrooms, or laboratories to help students construct, visualize, and manipulate objects in a physical representation (nonvirtual) three-dimensional (3D) space. According to the National Center for Education Statistics, there are roughly 26,000 High Schools in the United States¹ and approximately 4,000 colleges/universities.² Thus, a substantial cohort could benefit from the present model kit.

BACKGROUND

The present kit adheres to a paradigm of constructing a resilient molecular model system that helps visualize 3D-geometrical relationships, including the internuclear distances and the torsion angles between the atom nuclei in a molecule.³⁻⁵ This kit components relate to the field of molecular model systems and particularly to systems that include components molded from extruded thermoplastic filaments (such as polylactic acid (PLA)) sufficiently resilient to permit them to be interlocked firmly but in such a way that torsion angles of most functional groups can be rotated over a long service life without rapid wear or inadvertently falling apart after moderate use. The application of the model kit is to demonstrate concerted conformational changes in molecules related to rotational and torsional degrees of freedom about the bonds over a long service life.

DESIGN OBJECTIVES OF THE MODEL KIT

One objective is to provide a molecular model system comprising components that can be easily assembled to render a molecular model of practical accuracy (e.g., cycloalkane and short-chain alkane) and interlock while permitting parts or all of the model to rotate relative to other parts. The disassembly must also require minimum time. Another objective is to provide molecular model components that can be molded of inexpensive extruded polymeric material (such as PLA) to provide an economical model set (Table 1, Figure 1). Further objectives are apparent from the specifications and figures included below.

Table 1. Model Kit Components

Atom Representation	Filament Color	Number of Elements	Cost
Carbon	Black	10	\$5.04
Hydrogen	White, non-luminous 6 Blue/6 Green, luminous	22	\$4.36
		12	\$2.37
Bond	yellow, non-luminous, with steel rod inserts	32	\$18.00
Bond	6 Blue/6 Green, luminous, with steel rod inserts	12	\$6.95
Flexible Bond	yellow rod, non- luminous, without steel rod inserts	8	\$4.50
Coupler	White PTC	62	\$6.20
Packaging			\$5.00
TOTAL			\$52.42



Figure 1. The packaging contents are described in Table 1.

DETAILED DESCRIPTION OF THE INVENTION

The system includes components representing atoms/nuclei and other components serving as couplers between the atoms/nuclei for mechanical assembly but also representing bonds between atoms. Each component representing an atom is a 35 or 50-mm spheroid containing one to four push-to-connect (PTC) fittings with an externally threaded male end screwed into the threaded spheroid. The PTC fittings receive a shaft extending outwardly from the component corresponding to the atom. The shaft and axial length of the PTC fastener represent a bond between one atom and another, thus representing an approximately proportional

internuclear distance between two atoms of the molecular model. The PTC fastener is available from commercial suppliers (for example, APC, Malida, Dmfit, and Parker), and the general description and function of these connectors are included elsewhere.⁶

There is no difference between the shaft lengths on atom components representing specific chemical elements. Color coding of atoms is included per color standards for atoms: components representing carbon are colored black, and those representing hydrogen are colored white. However, the kit is extensible and can include atoms representing oxygen colored red and those representing nitrogen blue. Designer components such as atom representations branded with school colors, logos, or specialized luminescent colors (Figure 2) can also be included to stylize, emphasize, and contrast relative atom/bond positions.

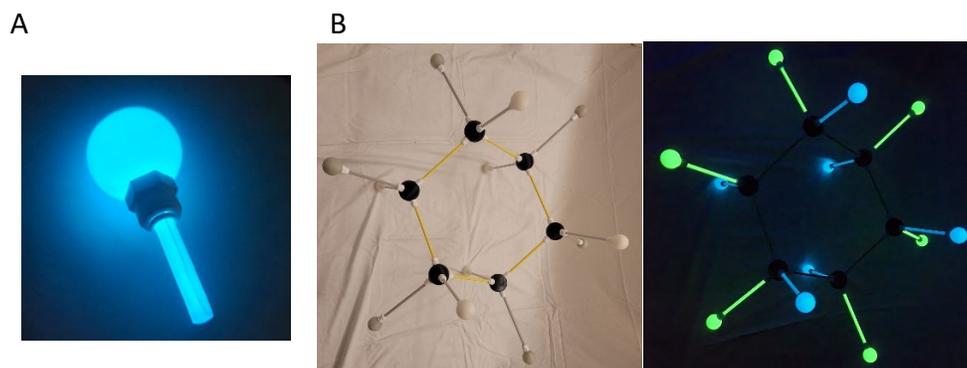


Figure 2. Atom representations printed with luminous PLA filament instead of a non-luminous filament, for example, A) a hydrogen atom and B) a cyclohexane molecule with C-H bonds at axial and equatorial positions. The printing parameters of these luminescent components are similar to those described below.

The carbon atom components are represented as tetravalent, containing four PTC fittings, each spaced 109.5° . Components representing atoms of other elements may have a different number of PTC fittings depending on the number of bonds that can be made with that atom in a particular model. For example, nitrogen atom components would be trivalent, containing three PTC fittings; oxygen atom components would be divalent, containing two PTC fittings. In this kit, hydrogen is monovalent, containing one PTC fitting. These atom components are the most commonly viewed in an Organic Chemistry course. Because the model kit is extensible, the hybridization geometries of a tetravalent sp or sp^2 atom can also be made.

Designing the Tetravalent Carbon Atom Representation. The 3D-modeling program Autodesk Fusion 360 (Mill Valley, CA) was used to design the spheroid representations of the tetravalent carbon. The "Create Solid Body Sphere" function was used to generate a 50 mm diameter sphere. The "Split Body" function was used to split the sphere into two equal hemispheres along the XY plane. Each of these hemispheres was made into individual components, and the bottom hemisphere body component was selected. Centered on the XY plane while using the "Center Diameter Circle" Sketch function, a 50 mm diameter circle was created at the intersection point of the X and Y axes relative to the axes of the sketch. Using the "Create Line" Sketch function, three 25 mm lines extending from the center of the sketched circle and separated 120° from each other were added. The "Create Line" function was also used to draw three 10 mm lines tangent to the circle and perpendicular to and centered on each of the 25 mm lines (Figure 3A). The "Plane Along Path" Construction-Plane function created three construction planes bisecting each of the 25 mm reference lines (Figure 3B).

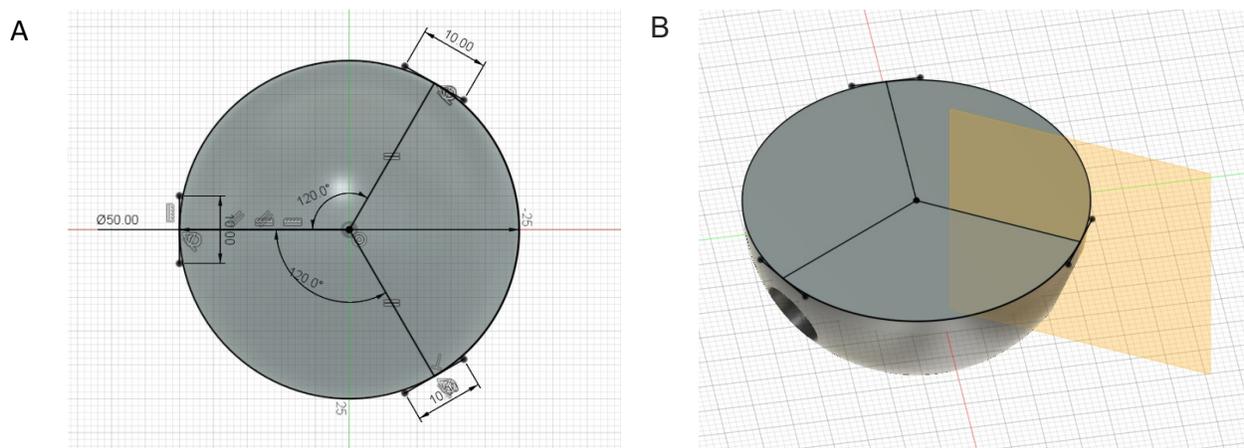


Figure 3. A) The bottom hemisphere of the tetravalent carbon atom representation with the reference angles placed in the XY plane by the Sketch function in the Fusion 360 program, and B) the placement of the construction plane to place the holes for the bond anchor points in the bottom hemisphere of the carbon atom representation.

A sketch was generated separately on each of the three bisecting construction planes. In this sketch, the "Create Point" Sketch function was used to insert two points on each edge of the flat surface of the bottom hemisphere body. The bottom hemisphere body needed to be visible in Sketch Mode for this step. A 50 mm line was drawn to connect the points using the "Create Line" function. A 25 mm line at 90° to the center of the 50 mm line was drawn with the "Create Line" function. A second 25 mm line was drawn from the center of the 50 mm line at 160.5° to the periphery of the bottom hemisphere body (Figure 4A). This sketch was repeated for the two

remaining construction planes bisecting the bottom hemisphere body (the planes referenced in Figure 1B). The "Plane Tangent to Face at Point" Construction Plane function was used to place a construction plane at the endpoints of the three 160.5° 25 mm lines (Figure 2B).

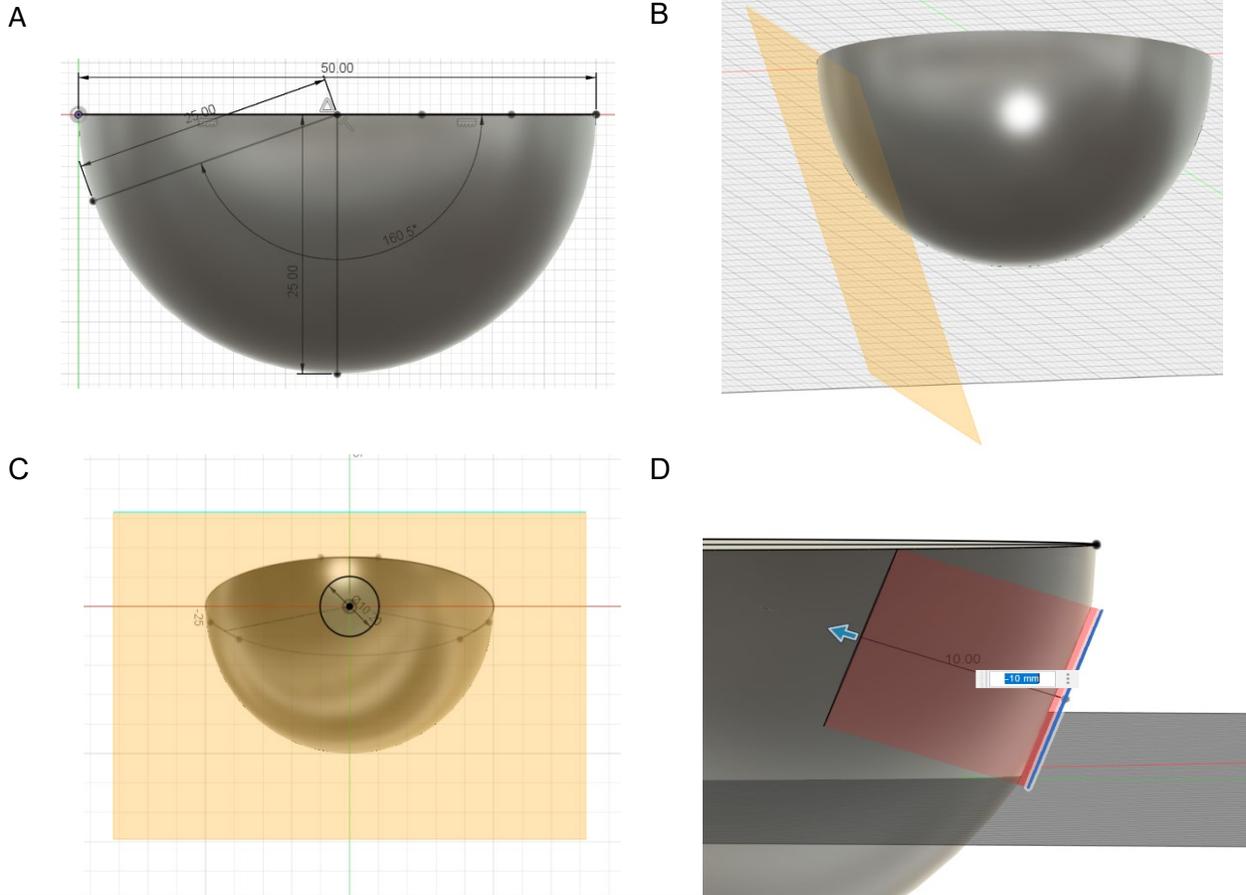


Figure 4. The bottom hemisphere of the tetravalent carbon atom representation in Sketch Mode shows A) the drill angle of one of the three holes acting as an anchor point in the carbon atom representation and B) the construction plane placement for inserting a hole at the correct location and angle (panel C shows the construction plane in panel B from a front-on vantage point). D) The hole extrusion for 1/8 inch NPT female thread x 10.2 mm depth represents one of three attachment points on the carbon atom; the +/- sign defines the extrusion direction in Fusion 360.

A sketch was generated on one of the construction planes, which are tangent to the bottom hemisphere face on the endpoint of the 160.5° 25 mm line. The "Create Center Diameter Circle" Sketch function was used to place a 10.2 mm x 10.2 mm length hole on the intersection point of the X and Y axes relative to the axes of the sketch (Figure 4C). Using the "Extrude" Body-Shaping function and the "Cut" operation of the "Extrude" function, the 10.2 mm circle was extruded 10.2 mm into the bottom hemisphere body to create the hole (Figure 4D). This process was repeated on the remaining two construction planes, which are tangent to the

bottom hemisphere face on the endpoint of the 160.5° 25 mm line. These steps created the receptacles for the bonds at the proper 109.5° for a tetravalent carbon atom representation.

Each 10.2 mm x 10.2 mm hole was threaded the entire depth with 1/8in NPT threads using the "Thread" function. The "Modeled" setting in the "Threads" function should be selected to ensure the threads can be exported from the Fusion 360 program.

Next, the top hemisphere component was selected in Fusion 360. Using the "Offset Plane" Construction Plane function, a construction plane was placed 25 mm from the XY plane and centered on the axis of the top hemisphere (Figure 5A, B). A sketch was created on the offset construction plane. The "Create Center Diameter Circle" Sketch function was used to place a 10.2 mm diameter x 10.2 mm length hole on the intersection point of the X and Y axes relative to the axes of the sketch. Using the "Extrude" Body-Shaping function and the "Cut" operation of the "Extrude" function, the 10.2 mm circle was extruded 10.2 mm into the top hemisphere body to create the fourth (top) hole (Figure 5C, D). The 10.2 mm x 10.2 mm hole was threaded the entire depth with 1/8 inch NPT threads using the "Thread" function. The "Modeled" setting in the "Threads" function should be selected to ensure the threads can be exported from the Fusion 360 program.

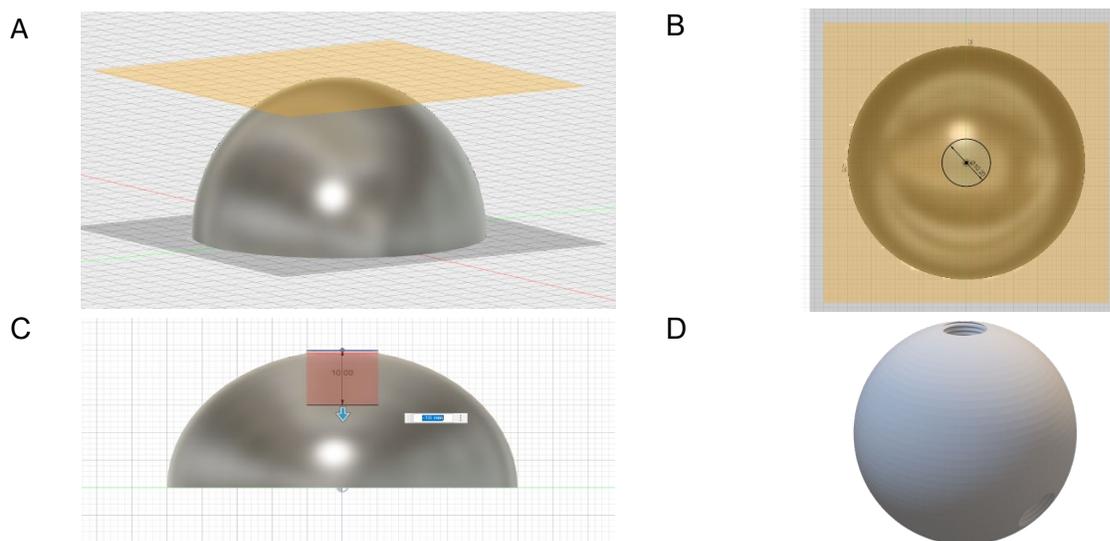


Figure 5. The top hemisphere of the tetravalent carbon atom representation in Sketch Mode shows A) the placement of the construction plane for designing the top hole, representing the fourth anchoring point (panel B shows the construction plane in panel A from a top vantage point). C) The hole extrusion for 1/8 inch NPT female thread x 10.2 mm depth represents the fourth attachment point on the carbon atom representation; the +/- sign defines the extrusion direction in Fusion 360. D) Closed shell stereolithography (STL) model of the tetravalent carbon atom (two of the four holes are visible).

Designing the Monovalent Hydrogen Atom Representation. The "Create Solid Body Sphere" function in Fusion 360 was used to generate a 35 mm diameter sphere. Using the "Offset Plane" Construction Plane function, a construction plane was placed 17.5 mm above the XY plane (Figure 6A). A sketch was placed on the offset plane. Using the "Center Diameter Circle" Sketch function, a 10.2 mm diameter circle was placed on the intersection point of the X and Y axes relative to the axes of the sketch (Figure 6B). Using the "Extrude" Body-Shaping function and the "Cut" operation of the "Extrude" function, the 10.2 mm circle was extruded 10.2 mm into the body to create the hole for the monovalent hydrogen atom representation (Figure 6C, D). The 10.2 mm x 10.2 mm hole was threaded the entire depth with 1/8 in NPT threads using the "Thread" function. The "Modeled" setting in the "Threads" function should be selected to ensure the threads can be exported from the Fusion 360 program.

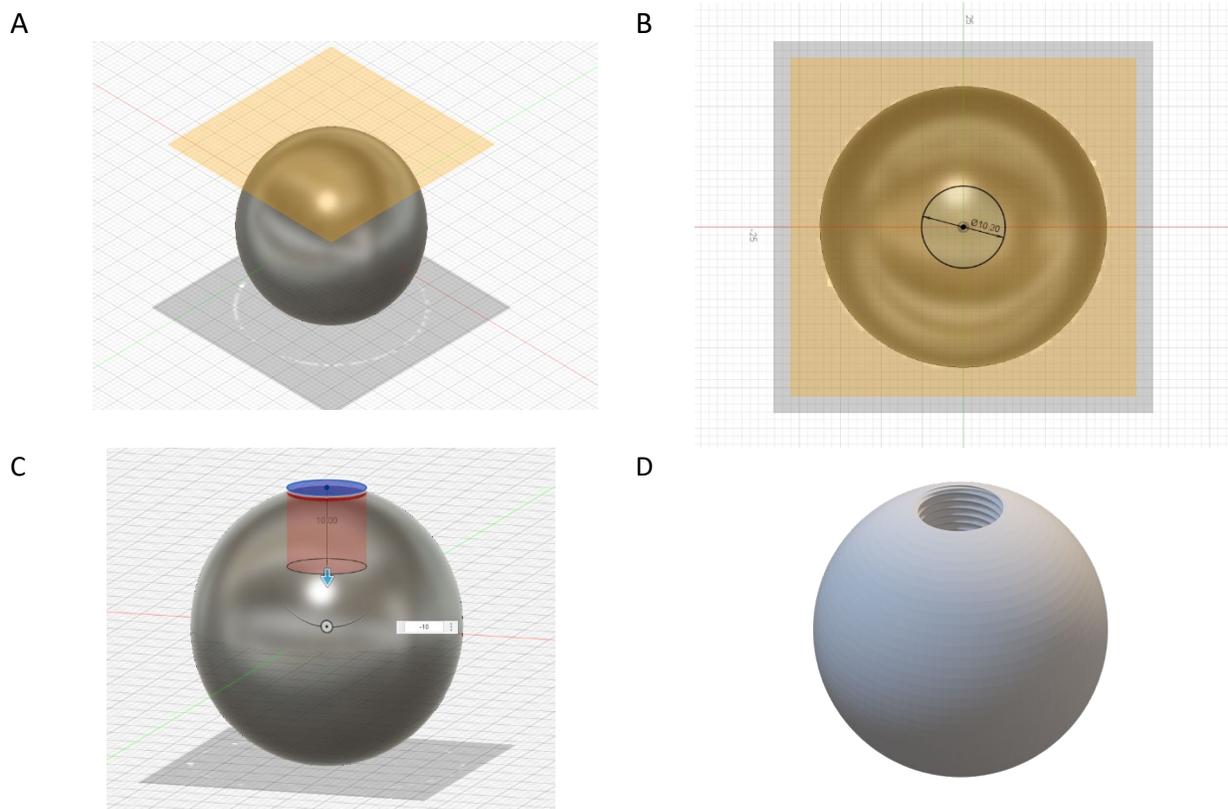


Figure 6. The sphere representation of the monovalent hydrogen atom in Sketch Mode shows A) the placement of the construction plane for designing the top hole, representing the anchoring point (*Panel B* shows the construction plane in *Panel A* from a top vantage point). C) The hole extrusion for 1/8 inch NPT female thread x 10.2 mm depth represents the attachment point on the hydrogen atom representation; the +/- sign defines the extrusion direction in Fusion 360. D) Closed shell stereolithography (STL) model of the monovalent hydrogen atom.

Exporting the Fusion 360 models to stereolithography (STL) files. Each of the Autodesk Fusion 360 designs was exported as an STL file for 3D printing.

Designing the Bond Representations. The 3D-modeling program FreeCAD ver 0.21.1 was used to design the bond representations for the molecular model.

Designing the Rigid-Bond Representations. Two concentric circles in the XY plane, the larger circle with a 6.5 mm diameter (OD) nesting an interior circle of 3.80 mm diameter, were generated with the "Create Sketch" function in FreeCAD. The concentric circles were extruded into a cylinder (155 mm) perpendicular to the XY plane with the "Pad" Part Design function. This design was exported as an STL file for 3D printing.

Designing the Flexible Bond Representation. A circle (6.5 mm) was generated in the XY plane using the "Create Sketch" function in FreeCAD. The circle was extruded into a rod (155 mm) perpendicular to the XY plane using the "Pad" function. This design was exported as an STL file for 3D printing.

3D Printing Filaments. Creality PLA filaments (1.75 mm diameter) were obtained from AMAZON LLC.

Constructing the 3D-printed atom and bond representations using PLA filament. A Creality Ender 3 S1 Pro (Shenzhen, China) was used to 3D print the atom representations. The Utilimaker Cura program version 5.5.0-beta.1 used the general settings to convert the STL files to G-code files that assign the XYZ-plane movement of the 3D printer as follows for PLA filament: layer height: 0.28 mm, line width and wall line width: 0.4 mm, wall thickness 0.8 mm, wall line count: 2, infill: 10% or 70%, infill pattern cubic, printing temperature: 215 °C, build plate temperature: 60 °C, print speed: 60 mm s⁻¹, and fan cooling 100%.

3D-printed carbon atom and hydrogen atom representations. A component that represents a tetravalent carbon atom was 3D printed with black PLA filament with 10% infill to create a 50-mm sphere containing four threaded (NPT 1/8 inch) holes equally spaced 109.5° (Figure 7A). One of four identical PTC fastener components (Figure 7B) was threaded into each hole.

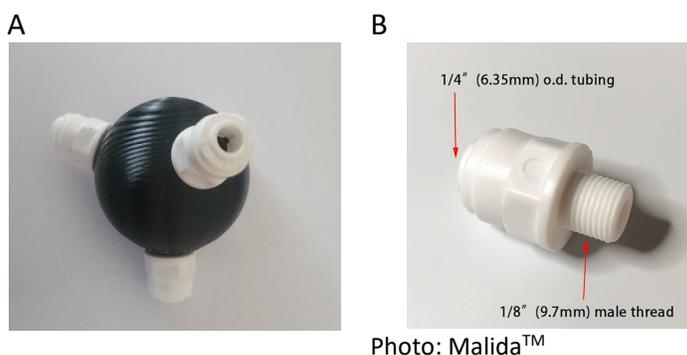


Figure 7. A) A 50 mm 3D representation of a tetraivalent carbon atom printed with black PLA filament fitted with B) push-to-connect (PTC) inserts threaded into each of the four holes of the carbon atom model in *Panel A*.

A component representing a monovalent hydrogen atom (Figure 8) was 3D printed with white PLA filament to create a 35 mm sphere containing one threaded (1/8 inch NPT) hole. One PTC fastener component (see Figure 7B) was threaded into the hole.



Figure 8. A 35 mm 3D representation of a monovalent hydrogen atom printed with white PLA filament fitted with a push-to-connect (PTC) insert (see Figure 9B) threaded into the hole in the hydrogen atom model.

3D-printed rigid-bond representations. A component representing a bond between two representations of atoms (Figure 9A) was printed with yellow PLA filament with 70% infill as a single cylindrical shaft (Figure 9B). A cold-roll insertion rod (3.2 mm diameter, 155 m length) was inserted into the shaft and glued in place with two-part J-B Weld 5 Minute epoxy adhesive to prevent flexion along the axial length of the tube representing the bond (Figure 9B). The tubular shaft diameter (6.5 mm) (Figure 9C) is slightly oversized compared to the collet flange diameter (6.3 mm) of the PTC fastener attached to the spheroid representing the atom. The oversized shaft presses against the collet tabs in the PTC adapter and is grabbed tightly by the rubber o-ring (Figure 9D). Together, these forces reduce the rotational movement of the model and allow it to adopt desired conformational geometries, such as in the cyclohexane and *n*-butane models (Figure 10).

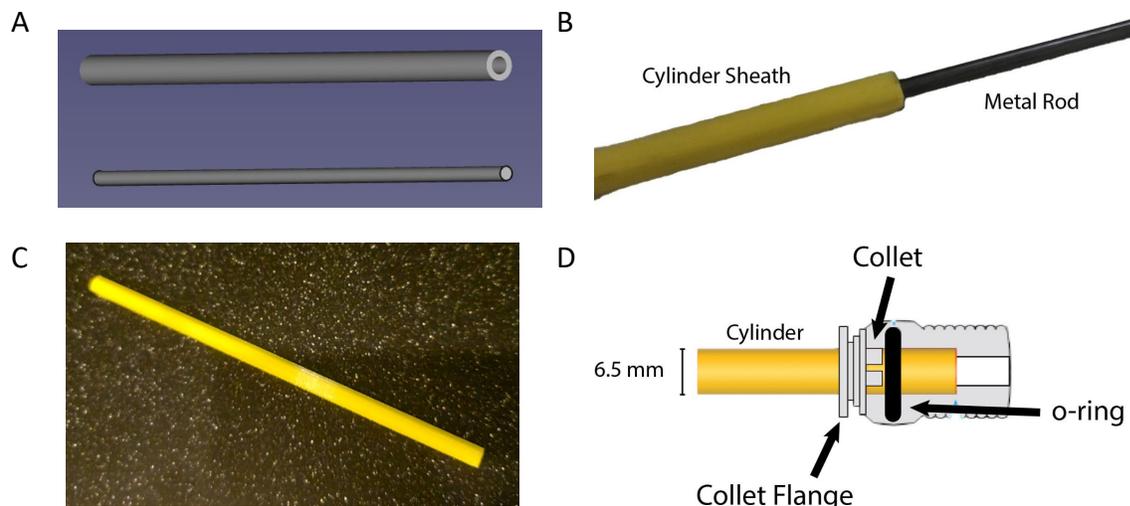


Figure 9. A) 3D-model renderings of the cylinder (OD: 6.5 mm; ID: 3.8 mm; L: 155 mm) and solid metal rod (OD: 3.2 mm; L: 155 mm) used to assemble the bond representations. B) The 3D representation of the cylinder printed with yellow PLA filament and the partially inserted and C) fully inserted cold-rolled metal rod. D) A cross-sectional rendering of the cylinder/rod representation of a bond fitted in a PTC fastener, highlighting how the components fit together: collet flange, collet, and rubber o-ring. Image adapted from the FiTAT company.

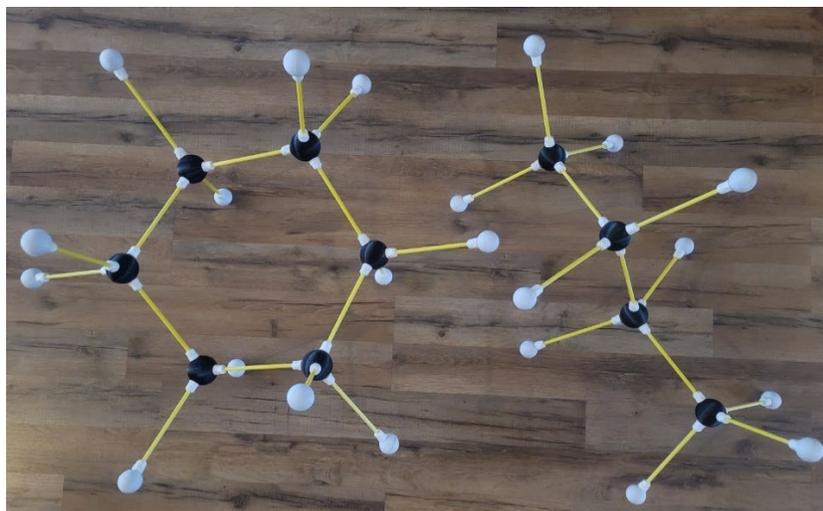


Figure 10. A model of *Left*) cyclohexane in a low-energy chair conformation and *Right*) *n*-butane in a staggered conformation using the components described in the current invention.

3D-printed flexible-bond representations. A flexible rod component representing an angle-strained bond between two representations of atoms was printed with yellow PLA filament with 70% infill (Figure 11A). The flexible rods are identical in length and diameter to the hollow PLA shafts containing the metal insertion rod (see Figure 9), except they are closed-end, made entirely of extruded plastic, and do not contain a metal insertion rod.

These flexible rods create cyclohydrocarbon structures comprising tetrahedral atoms with bonds exhibiting angle strain with bond angles $<109.5^\circ$. These specialized cylinders give the instructor or student access to, for example, cyclopropane to demonstrate the inherent ring strain (i.e., angle strain) in the cyclic structure by viewing the flexion in the shaft, which gives a visible representation of the strained condition (Figure 11A). The ring strain in cyclobutane, which uses the representation of four tetrahedral atoms, is also visible in a strained parallelogram model (Figure 11B).

Since the model kit is intended for demonstrations in a sizeable instructional setting, the shafts representing bonds are the same lengths, for example, for the C-C and C-H bonds. Thus, they represent between 1.00 and 1.25 cm \AA^{-1} to highlight the relative dihedral angles between the bonds represented by the shafts and the location and orientation of the atoms resulting from a change in the bond angles. Also, the relative diameters of the atoms, such as those in the second row of the periodic table, and hydrogen are sized for visibility and to roughly illustrate the relative van der Waal radii for the atoms represented.

The resulting skeletal structures will provide a 3D model of the stick structure conventions used when drawing skeletal (or line bond) structures for organic chemistry molecules. These models give the learner or instructor a tactile model to aid in understanding the conformational dynamics and intramolecular steric interactions crudely represented by static 2D drawings typically used to convey organic chemistry structures.

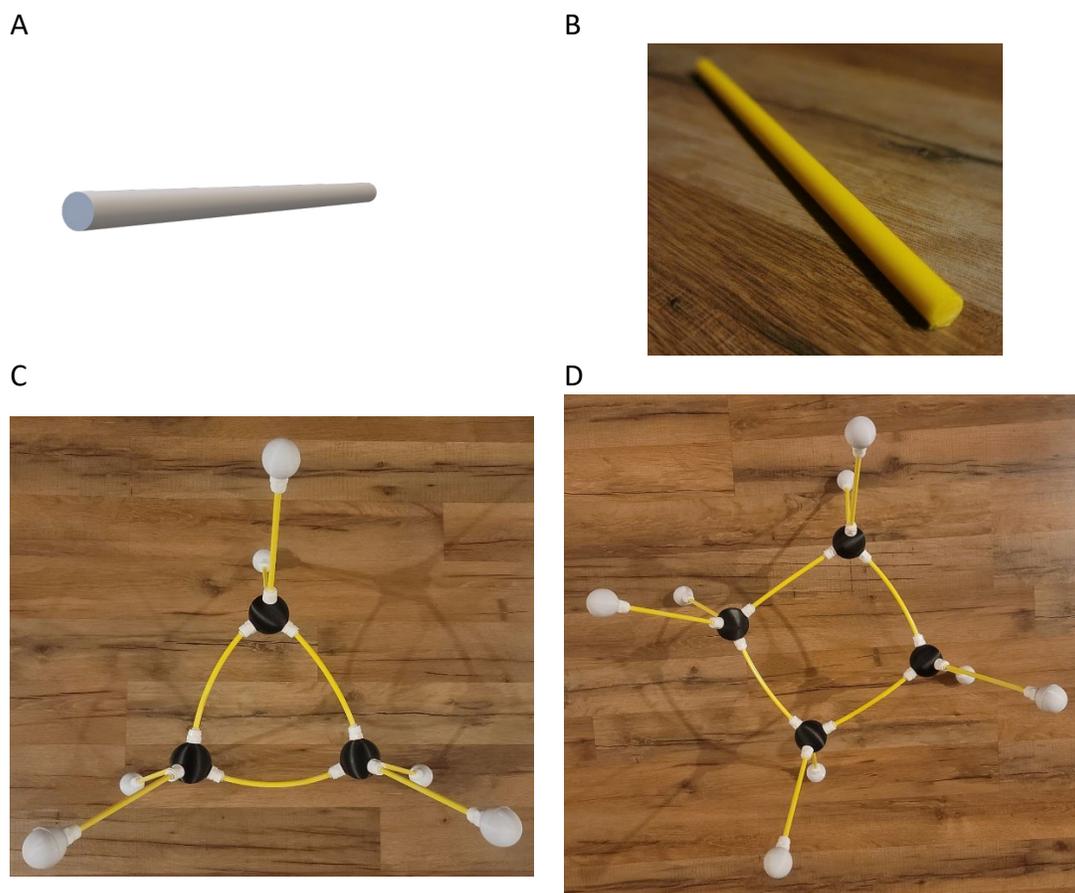


Figure 11. A) 3D-model renderings of the PLA rod (OD: 6.5 mm; L: 155 mm) used for the flexible bond representations. B) The 3D representation of the 3D cylinder printed with yellow PLA filament. Applying the flexible bond representations in a representation of C) cyclopropane and D) cyclobutane.

BENEFITS OF THE DESIGN

Model Disassembly. Disassembly of the shafts representing the bonds from the PTC fastener attached to the spheroids representing atoms is done with an inward force on the collet flange by a flathead screwdriver or equivalent and an outward force on the shaft (usually applied by hand) when a different molecular model configuration is desired.

Model Serviceability. Additional benefits of the current invention are that components can be maintained with nonproprietary replacement parts, such as standard plumbing o-ring (Danco 96715) within the PTC coupler that provides rotational friction. Also, the threaded PTC couplers can be unscrewed and replaced if necessary.

Application of PLA for Bioremediation and Recycling. The PLA used to make a majority of the model kit is a recyclable biopolymer made from renewable plant-based feedstocks (sugar beets, sugar cane, wheat, or corn), and it can be broken down in a few months by microorganisms with controlled temperature, humidity and microorganisms at an industrial composting facility.⁷

The PLA recycling stream needs high-quality material; thus, the current model is adhesive-free, ensuring the PLA used in the model kit is contaminant-free for potential recycling after service. The conscious effort to reduce contamination also makes the PLA used here suitable for chemical recycling, where the polymer is hydrolyzed into its monomers that can be used to produce new PLA.⁸

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