3D-Printed Models for Explaining Organic Chemistry Concepts

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Introduction

Three dimensional models allow students to better visualize a concept with the ability to physically hold and rotate the object in their hands. This hands-on learning through 3D printing has been used to teach chemistry concepts. For example, 3D printed models have been used to teach symmetry and point groups in inorganic chemistry,[1-2] potential energy visualizations,[3-4] and even protein models[5]. Davidson professors Felix A. Carroll and David N. Blauch have used 3D-printed models to visualize structure-energy relationships and energy pathways in S_N2 and S_N1 reactions.[6] This investigation applies 3D printing to explain other organic chemistry concepts. 3D models were developed to show an internal plane of symmetry with the aid of a mirror to show the S_N2 reaction of a nucleophile attacking an unhindered alkyl halide.

3D Printing Background

3D printing is an additive process that follows a few universal steps:

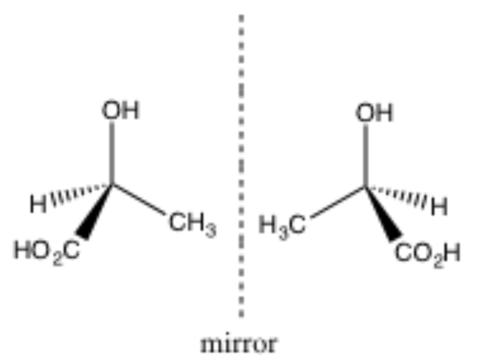
1. The object to be printed is designed on a computer using CAD (computer-aided design) software.
2. The model is converted to a .stl (stereolithography) file which is a mesh made of triangles and the language understood by 3D printers.[3]
3. The 3D printer constructs the object by adding one layer of material on top of another as the print bed lowers.
4. The model is post-processed, which could include removing supports, sanding, painting, or gluing.

Various types of 3D printing exist, and they differ in the type of material used, speed of printing, and the resolution of the solid produced:

- **Stereolithography** uses a laser beam and photopolymer resins.
- **Laser sintering** uses a laser to fuse powder into a solid object.
- **Digital light processing** uses light to build an object out of photopolymers.
- **Inkjet** 3D printing uses an inkjet to bind powder into a solid.[7]
- **Fused filament deposition** (FFD) is the type of printing that was used in this project. In this method, an extruder heats and melts plastic filament that is added on, layer by layer, to form a design, using fans to harden the plastic right after deposition.[7] Fused filament deposition is useful because it's fast, the PLA filament is cheap, and design customization is easy.[8]

Achiral Model

A molecule is achiral if it has an internal plane of symmetry, as shown below.

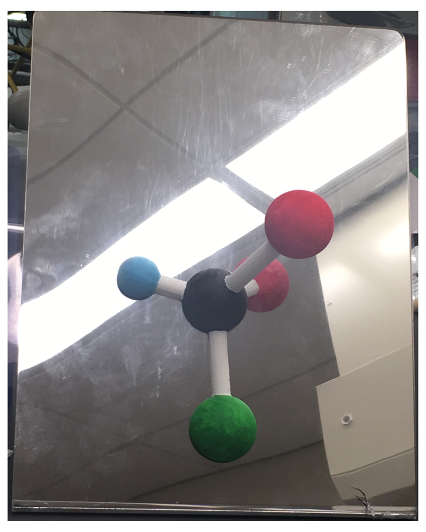


Spartan '16 was used to create the model of the achiral organic molecule and convert it to a .pdb file. *Visual Molecular Dynamics (VMD)* was used to adjust the representation of the molecule using the van der Waals (VDW) and space-filling (CPK) settings according to Table 1. The model was rendered as an .stl triangle mesh file. *netfabb* was used to repair the model, measure and adjust the scale of the molecule so each atom could hold a 18 mm diameter magnet, split the model in half, and create the mirror image of the half of the molecule. *Meshmixer* was used to convert the from a mesh to a solid. *123D Design* was used to create holes in the atoms for magnets by placing a cylinder with the same diameter and height of a magnet inside the atom and subtracting the cylinder. Within *Makerbot Desktop*, the settings were adjusted to create a raft and supports for the model, set the infill to 15%, rotate the molecule, and export the .stl file as an .x3g file that was printed on the *Makerbot Replicator 2*. After printing the molecule, the raft and supports were removed, the model was smoothed down with a sanding tool and painted with acrylic paint, and the magnets were superglued into the holes.

Table 1. Achiral Molecule Representation Settings in VMD

Representation	Sphere Res.	Bond Res.	Bond Radius	Sphere Scale
VDW	50	–	–	0.3
CPK	50	50	0.5	0.1

Models of half of a molecule and its mirror image with magnets that could be attached to a mirror were produced and are shown below. Pulling the halves up and off the mirror together with an acetate sheet in between helps explain visually how a molecule is achiral if it has an internal plane of symmetry.



S_N2 Space-filling Models

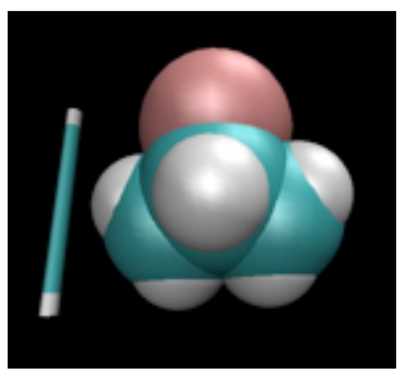
In a S_N2 reaction, a nucleophile (1) will only attack an unhindered alkyl halide (2), as shown below.

1 2

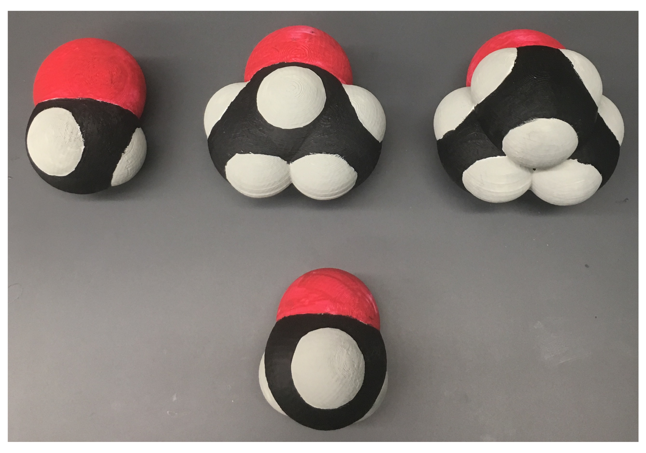
The molecular models were designed with space-filling representation settings in *Spartan '16*. In order to simulate this space-filling representation in *VMD*, the sphere scale was enlarged. The molecules were scaled to the same size by creating a model of 1,3-butadiyne in *Spartan '16* that mimicked a ruler and served as a point of reference. The 1,3-butadiyne was grouped with each alkyl halide model in *VMD*, as shown below, and the CPK settings were adjusted according to Table 2. Once rendered as an .stl file, the scale of the model was adjusted in *Autodesk Fusion 360* to enlarge the 1,3-butadiyne ruler to a constant length which simultaneously scaled the alkyl halide model to a constant size. The *Autodesk Fusion 360* file was sent to *Meshmixer* and exported as a .stl. The .stl file was opened in *netfabb* and the 1,3-butadiyne ruler was removed by selecting and deleting the shells. The file was exported to *Makerbot Desktop* and printed as an .x3g file from the *Makerbot Replicator 2* with a raft, supports, and 15% infill. Once printed, the support and rafts were removed and the models were smoothed down and painted with acrylic paint.

Table 2. CPK Space-filling Representation Settings in VMD

Model	Sphere Res.	Bond Res.	Bond Radius	Sphere Scale
1,3-butadiyne	50	50	0.9	0.2
Alkyl halide	50	50	0.3	6.0



Models of the nucleophile (methoxide, on bottom) and three alkyl halides with different sterics (from left to right: methyl bromide, isopropyl bromide, and *tert*-butyl bromide) were produced. The models provide first-hand understanding of why a S_N2 reaction will not work with a sterically hindered alkyl halide – the methoxide cannot physically get to the carbon because the methyl groups are in the way.



Acknowledgment

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References

1. Scalfani, V.F.; Vaid T.P. 3D Printed Molecules and Extended Solid Models for Teaching Symmetry and Point Groups. *J. Chem. Educ.* **2014**, *91*, 1174–1180.
2. Casas, L.; Estop, E. Virtual and Printed 3D Models for Teaching Crystal Symmetry and Point Groups. *J. Chem. Educ.* **2015**, *92*, 1338-1343.
3. Lolur, P.; Dawes, R. 3D Printing of Molecular Potential Energy Surface Models. *J Chem. Educ.* **2014**, *91*, 1181-1184.
4. Teplukhin, A.; Babikov, D. Visualization of Potential Energy Function Using an Isoenergy Approach and 3D Prototyping. *J. Chem. Educ.* **2015**, *92*, 305-309.
5. Meyer, S.C. 3D Printing of Protein Models in an Undergraduate Laboratory: Leucine Zippers. *J. Chem. Educ.* **2015**, *92*, 2120-2125.
6. Blauch, D.N.; Carroll, F.A. 3D Printers Can Provide an Added Dimension for Teaching Structure-Energy Relationships. *J. Chem. Educ.* **2014**, *91*, 1254-1256.
7. 3D Printing Industry. 3D Printing Processes. http://3dprintingindustry.com/3d-printing-basics-free-beginners-guide/processes/ (accessed Mar 2, 2017).
8. SD3D Printing. FFF vs. SLA vs. SLS: 3D Printing. http://www.sd3d.com/fff-vs-sla-vs-sls/ (accessed Mar 2, 2017).