

3D Printed Models for Chemical Education

Tamara Ilioska,¹ Jan Hočevar,¹ Martin Rihtaršič,¹ Aleš Mavsar,² Jasna Zabel,³ Žan Mole,³ Erik Kerpan,³ Jan Koler,¹ Janja Pust,⁴ Marica Starešinič,³ Jernej Iskra*¹

¹Faculty of Chemistry and Chemical Technology, University of Ljubljana, ²Faculty of Education, University of Ljubljana,

³Faculty of Natural Sciences and Engineering, University of Ljubljana, ⁴Novo mesto Grammar School

*Corresponding author: jernej.iskra@fjkt.uni-lj.si

INTRODUCTION

Molecular models are indisputably the tool chemistry lecturers turn to for help when it comes to three-dimensional representation of chemical structures. Due to its affordability and commercial availability, 3D printing has become the best tool for making ideas come to life. We designed and 3D printed molecular models to be used as an educational tool for teachers and students. The design is based on the traditional ball and stick models with an interesting twist – use of magnets for atom-bond connection. The models improve visualization, resolve misconceptions, and increase understanding of chemical concepts.

CHARACTERISTICS

Size & Visualization

Big atoms. Appropriate for use in classrooms.

Realistic size ratios. Accurate depiction of atom sizes.



Magnetic bonding

+ **Durability.** No mechanical weakening of bonds.
↓ **Assembly time.** Simple to use, quick to assemble.

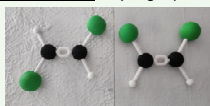
⊖ **Chemical bond concepts.** Bond formation is spontaneous and releases energy.



Left: sp hybridized C-atom. The bond hole includes two small gaps. Right: The gaps are complemented by a pair of matching protrusions at either end of the double bond.

Restricted double bond rotation

cis/trans isomerism. Easy to grasp the concept.



Axial chirality

A fine example of *axial chirality*. Cumulens perpendicular double bonds prevent rotation.

Cyclohexane conformation

Quick interconversion between axial and equatorial substituents.



Free rotation of the single bond

Free rotation around the single bond enables conformer visualization.



Bond length

Optical illusion. Triple bond appearing shorter than the single bond, despite being of same length.

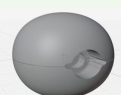


DESIGN

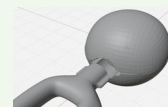
The models were designed to be visible across the lecture hall and to display the substantial differences in atom sizes.



Blender, a free and open code software, was used for modelling. We created a divider for the bond holes. The divider holds the magnet in place.



Two bond holes in a sp hybridized C-atom have a pair of small gaps to prevent rotation. The gaps are perpendicular, so that cumulated double bonds have correct 3D structure.



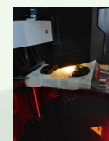
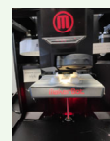
Bond formation is spontaneous and accompanied by the release of energy (as sound, whereas bond dissociation requires energy (physically pulling atoms apart)).



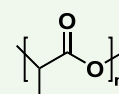
Before the two halves of each atom were glued together, magnets were inserted into the designated holes. Visible in the picture are three (out of the total four) magnets inside a nitrogen atom.



The design of the double and triple bonds creates an interesting optical illusion that double and triple bond appears shorter than the single bond despite having the same length.

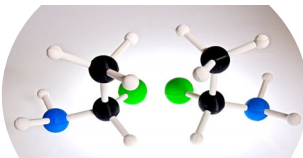


3D printer of choice: **MakerBot Replicator Mini**



3D printing material of choice: **polylactic acid (PLA)**

KLIKem

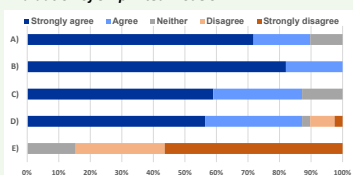


3D printed molecular models for improved visualisation of chemical concepts!

FEEDBACK

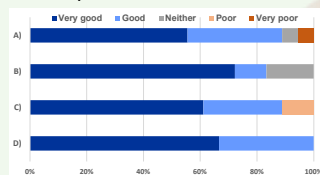
A survey questionnaire was compiled to ensure we have optimized the practicality, accuracy and presentability of the model set. The survey was conducted at Novo mesto Grammar School in September 2020. The survey involved 39 3rd year students.

Evaluation of 3D printed models:



- A) 3D printed models represent well the size of atoms
B) Assemblage of molecules is easy with 3D printed models
C) 3D printed models helps to visualize molecules better than other models
D) It is easier to see 3D structure of molecules with 3D printed models
E) I do not see differences between both sets

Students' questionnaire:



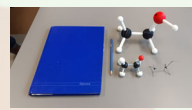
- A) Did making a 3D model of molecule help in understanding that energy is needed to break a bond?
B) How is your understanding of the size of the atoms in a molecule after making 3D models?
C) Did you get a good understanding about the rotation around single/double/triple bonds?
D) Did making a 3D model of molecule help in understanding the shape of a molecule?



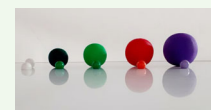
The constant communication with students helped us refine the models' design. Students tested the final model set and their positive feedback shows that our molecular models successfully bring 3D visualization of atoms closer to students.

CONCLUSION

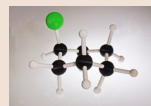
We designed a 3D printed, practical and intuitive chemistry set with magnetic bonding to be used as a pedagogical tool. The set utilizes:



- **Scaled up atoms and bonds** – for presentation of chemical concepts in a classroom or auditorium.



- **Atoms' experimental covalent radii** – for displaying the substantial differences in atom sizes.



- **Magnetic bonding** – for making quick and sturdy atom-bond connections, increasing set's longevity and durability.



- **Optimized design** – for explaining *cis-trans* isomerism in a classroom, especially in contrast with **conformational isomerism**.



- The concept that bond making releases energy and bond breaking requires energy.



- **Optical illusion** making double and triple bond appear different in size.

REFERENCES

- 1.C. Meinel, Models: Molecules and Croquet Balls. In: Models: The Third Dimension of Science, S. de Chadarevian, N. Hopwood (eds.), Stanford University Press, Stanford, California, 2004, 242-75.
2.C. E. Dickenson, R. A. R. Blackburn, R. G. Britton, 3D Printing Workshop Activity That Aids Representation of Molecules and Student Comprehension of Shape and Chirality. *J. Chem. Educ.* 2020, 97, 10, 3714-3719.
3.J. P. Brannon, I. Ramirez, D. Williams, G. A. Barding Jr., Y. Liu, K. M. McCulloch, Teaching Crystallography by Determining Small Molecule Structures and 3-D Printing: An Inorganic Chemistry Laboratory Module. *J. Chem. Educ.* 2020, 97, 2273-2279