Supplementary Information

Three-Dimensional Printing of a Scalable Molecular Model and Orbital Kit for Organic Chemistry Teaching and Learning

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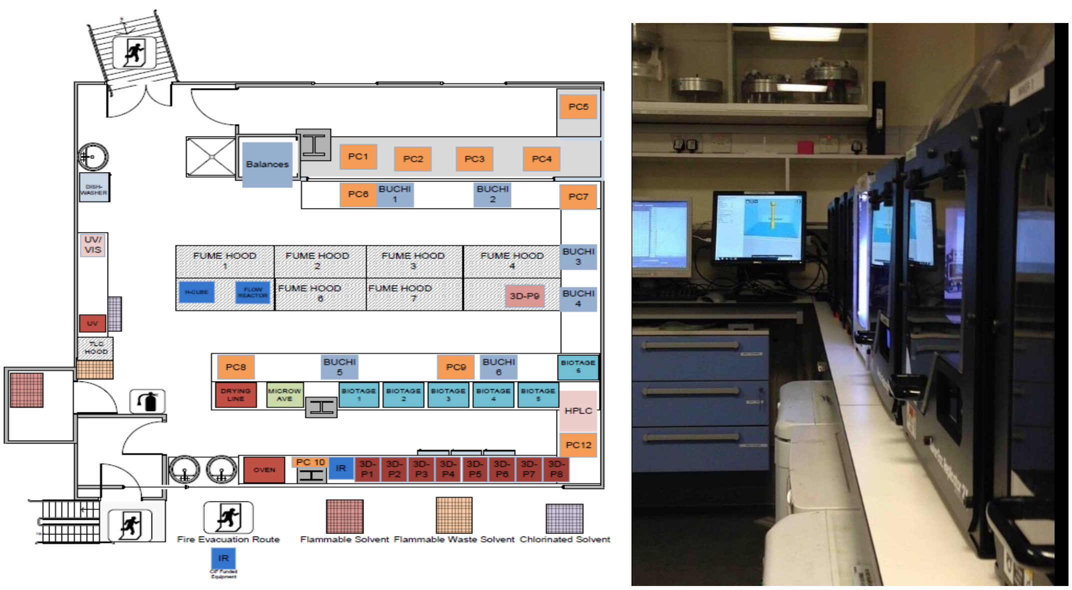
Contents

Infrastructure

A range of 3D printers was purchased for this study - comprising three MakerBot Replicator 2Xs, four MakerBot Minis and one Ultimaker 2 as we wanted to be able to simultaneously print a number of objects in a range of colours, explore a range of materials and, in the longer-term, utilise two-colour printing for alternative applications. All 3D printers (Supplementary Figure 1) were connected to a single PC (Windows 7, 64 Bit) located in a laboratory. This PC was then accessible via the network to the linked PCs in the laboratory. The aim of this was to explore the opportunity to connect via a PC microenvironment model of the department, with a host server running either MakerBot Desktop software or Cura as the controller for the 3D printers. The software was used to slice the .stl files prior to printing and to reduce preparation time.

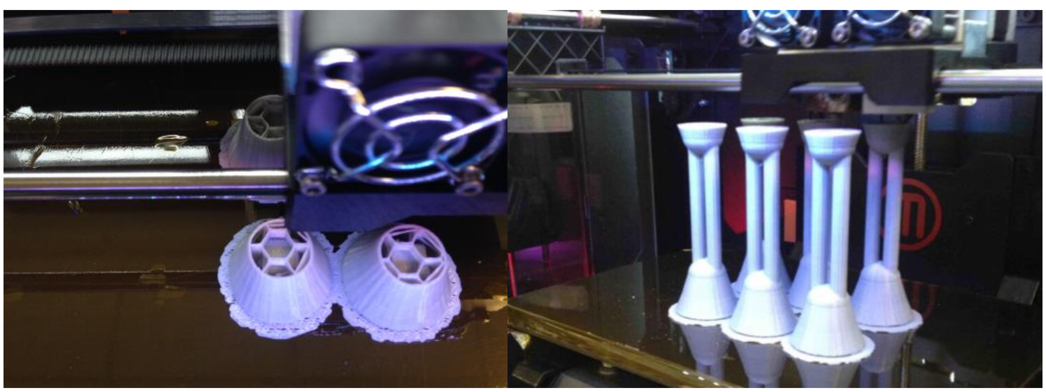


Supplementary Figure 1. Layout and plan of the laboratory showing the central location and arrangement of the 3D printers – 3D-P1 to P9.

Model Design and Printing

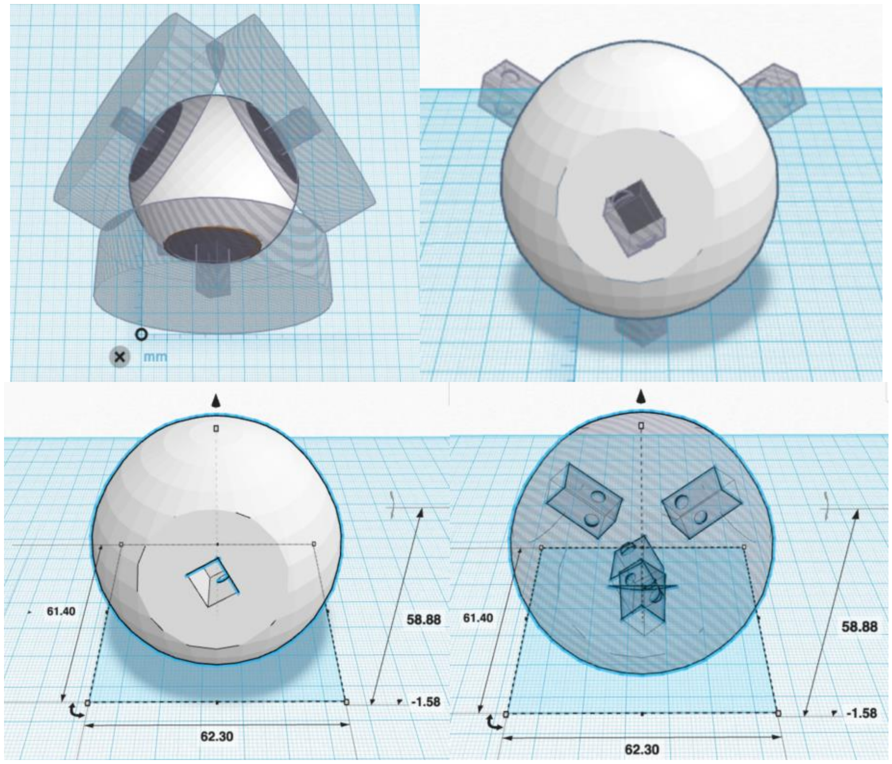
3D models of atoms, bonds and orbitals were designed using the browser-based 3D design tool - Tinkercad (www.tinkercad.com). Designs were developed via combinations of a range of shapes to create those shown in the following diagrams. The account used with this approach was linked to the corresponding author's account on Thingiverse (www.thingiverse.com), in order to facilitate the ready transfer of models to the printing process and program. Once designed, they were uploaded as .stl files and then prepared for printing using MakerBot Desktop.

Slicing of the models was carried out using MakerBot Desktop and models were printed using a raft, without supports and at 10% infill as shown below in order to reduce the weight and amount of plastic used (unless otherwise stated in each design). Designs were printed without support to avoid post-processing after printing. Multiple copies were also produced on a single build plate in order to reduce printing time (Supplementary Figure 2).



Supplementary Figure 2. Illustration of the 10% infill of models to reduce plastic use and weight (left) and the printing of multiple models in the same build (right).

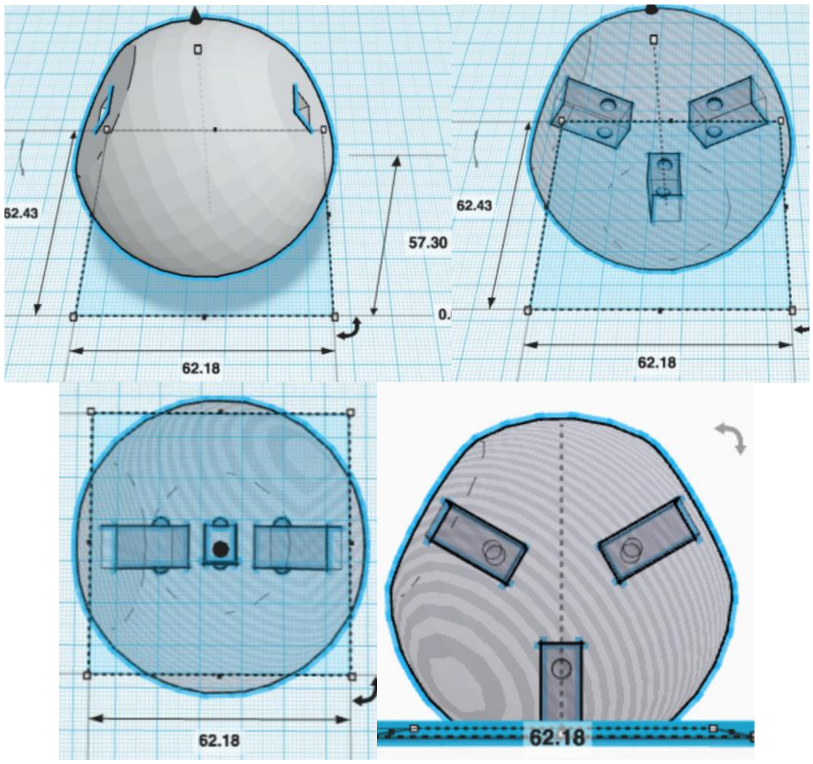
sp^3 carbon atom showing the iterative design process and final shape



Supplementary Figure 3. Model of sp^3 atom.

Infill Percentage:	10%
Material:	ABS/ PLA
Total Weight:	20.92 g
Cost estimate:	$ 0.55

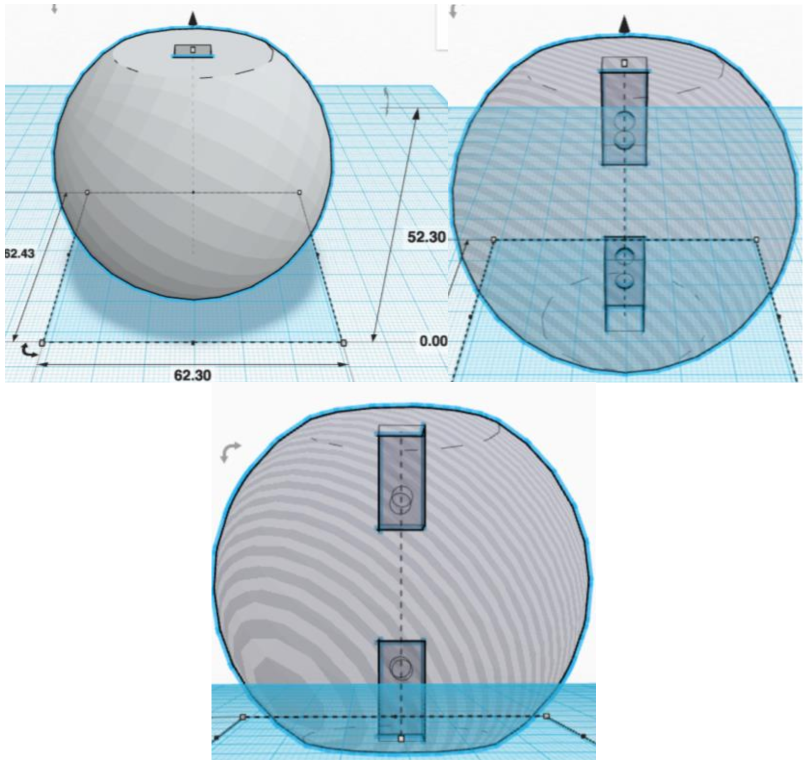
sp^2 carbon atom



Supplementary Figure 4. Model of sp^2 atom.

Infill Percentage:	10%
Material:	ABS/ PLA
Total Weight:	20.70 g
Cost estimate:	$ 0.55

sp carbon atom



Supplementary Figure 5. Model of sp atom.

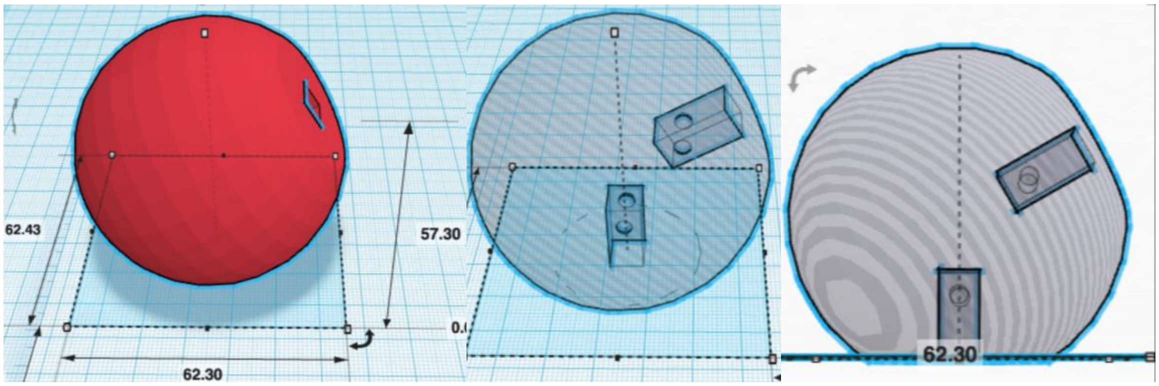
Infill Percentage: 10%

Material: ABS/ PLA

Total Weight: 20.27 g

Cost estimate: $ 0.53

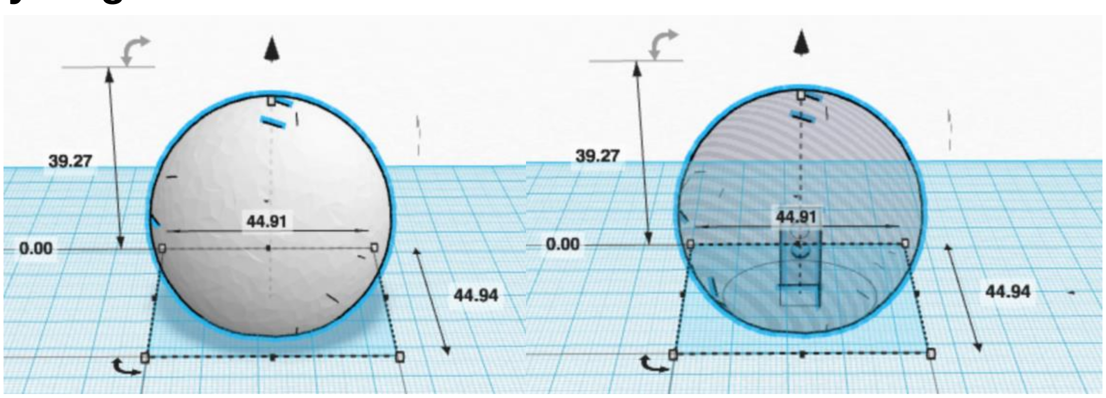
Oxygen atom



Supplementary Figure 6. Model of oxygen atom.

Infill Percentage:	10%
Material:	ABS/ PLA
Total Weight:	20.30 g
Cost estimate:	$ 0.53

Hydrogen atom

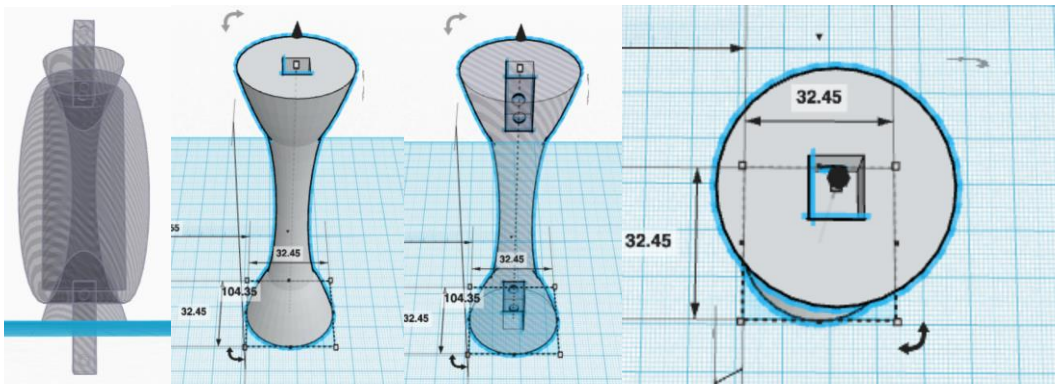


Supplementary Figure 7. Model of hydrogen atom.

Infill Percentage:	10%
Material:	ABS/ PLA
Total Weight:	9.10 g
Cost estimate:	$ 0.25

Single bond

This was developed via the combination of a number of shapes to provide a central thin solid core linked to two cones and smoothed out using elongated doughnuts as hollow subtractions to connect to the atoms described later. As can be seen below, the subtraction of the elongated tubes provided the curved shape to the single bond. Negative images of the clips provided the connection points on the bond.



Supplementary Figure 8. Model of single bond.

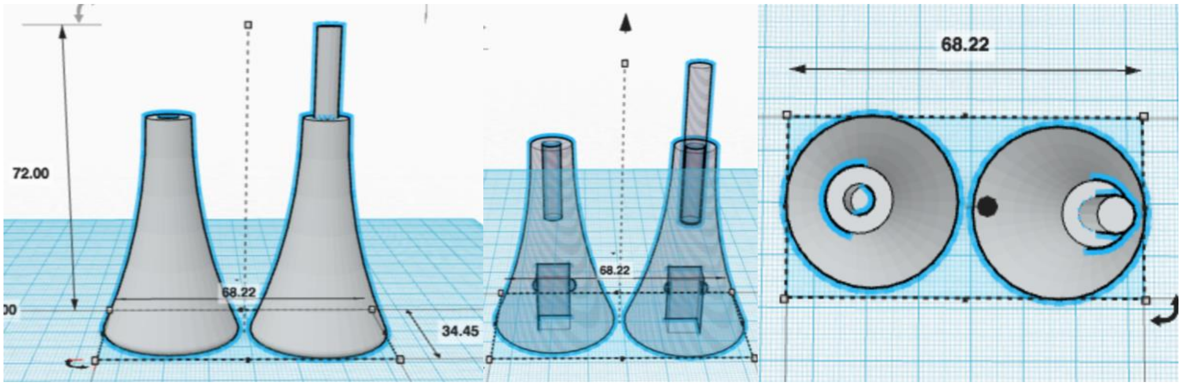
Infill Percentage: 20%

Material: ABS

Total Weight: 10 g

Cost estimate: $ 0.26

Rotatable bond



Supplementary Figure 9. Model of rotatable bond.

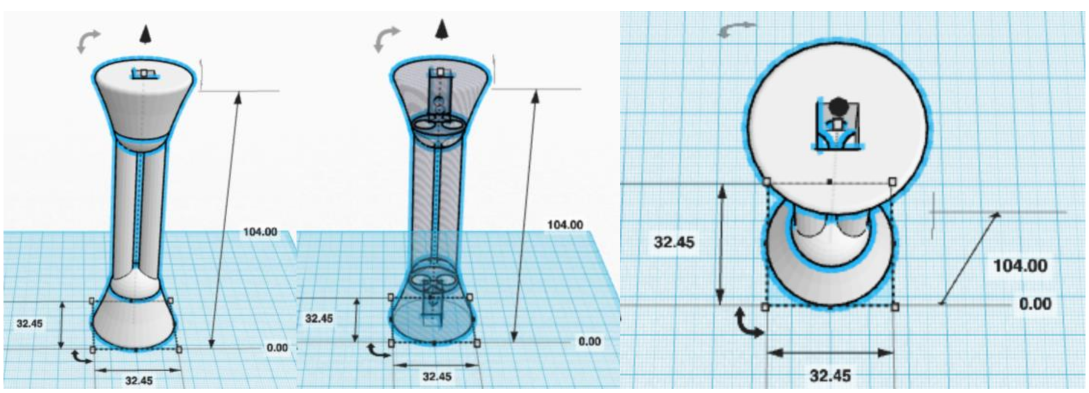
Infill Percentage: 30%

Material: ABS

Total Weight: 10.20 g

Cost estimate: $ 0.27

Double bond



Supplementary Figure 10. Model of double bond.

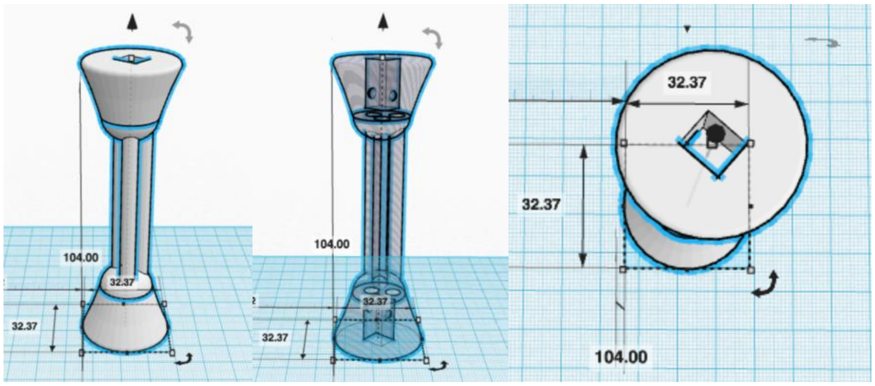
Infill Percentage: 20%

Material: ABS

Total Weight: 9.90 g

Cost estimate: $ 0.26

Triple bond

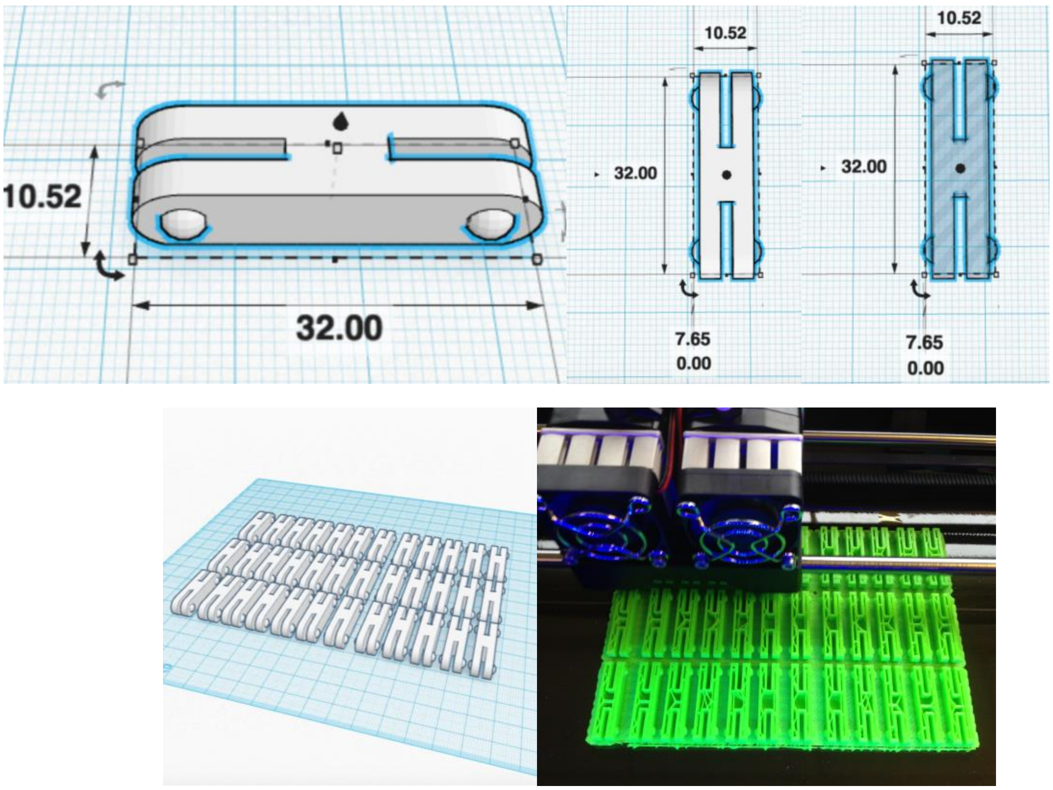


Supplementary Figure 11. Model of triple bond.

Infill Percentage:	20%
Material:	ABS
Total Weight:	10.20 g
Cost estimate:	$ 0.27

Clips for connection of atoms to bonds and orbitals

Multiple copies of the clips were printed in a single print in order to have sufficient quantity for assembly of the models.

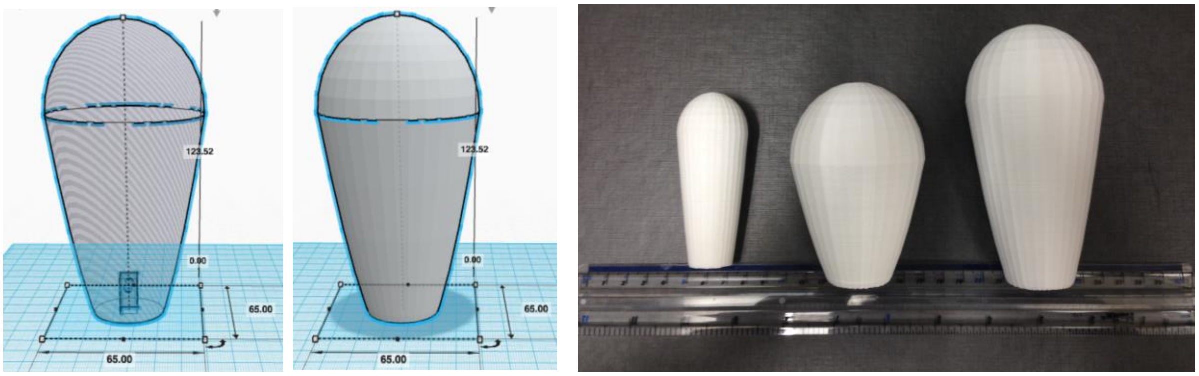


Supplementary Figure 12. Clip model.

Infill Percentage:	10%
Material:	ABS
Total Weight:	1.10 g
Cost estimate:	$ 0.03

Development of lone pair/ orbital

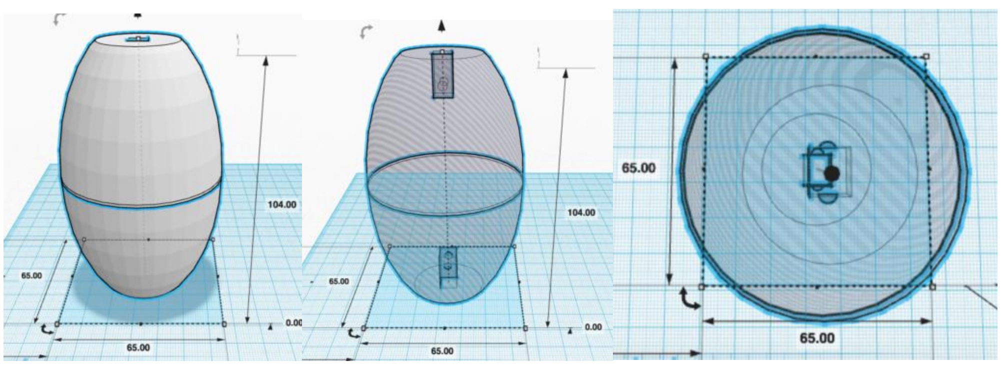
As can be seen below, a range of sizes for the printed lone pair were investigated to ensure that it was representative in the actual model, but also visible from a distance.



Supplementary Figure 13. Model of lone pair.

Infill Percentage:	10%	**Material:**	ABS Plastic
Total Weight:	56.83 g	**Cost estimate:**	$ 1.49

Development of sigma bond



Supplementary Figure 14. Model of sigma bond.

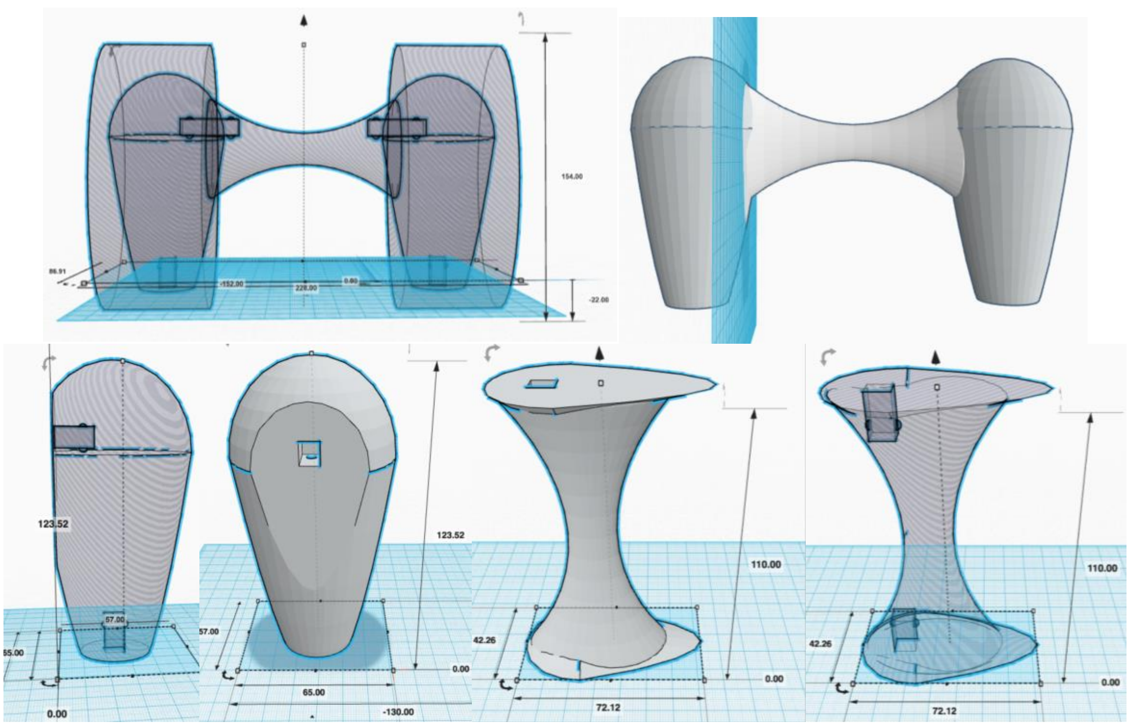
Infill Percentage: 5%

Material: ABS/ PLA

Total Weight: 34.52 g
Cost estimate: $ 0.91

Development of pi orbital model lone pair

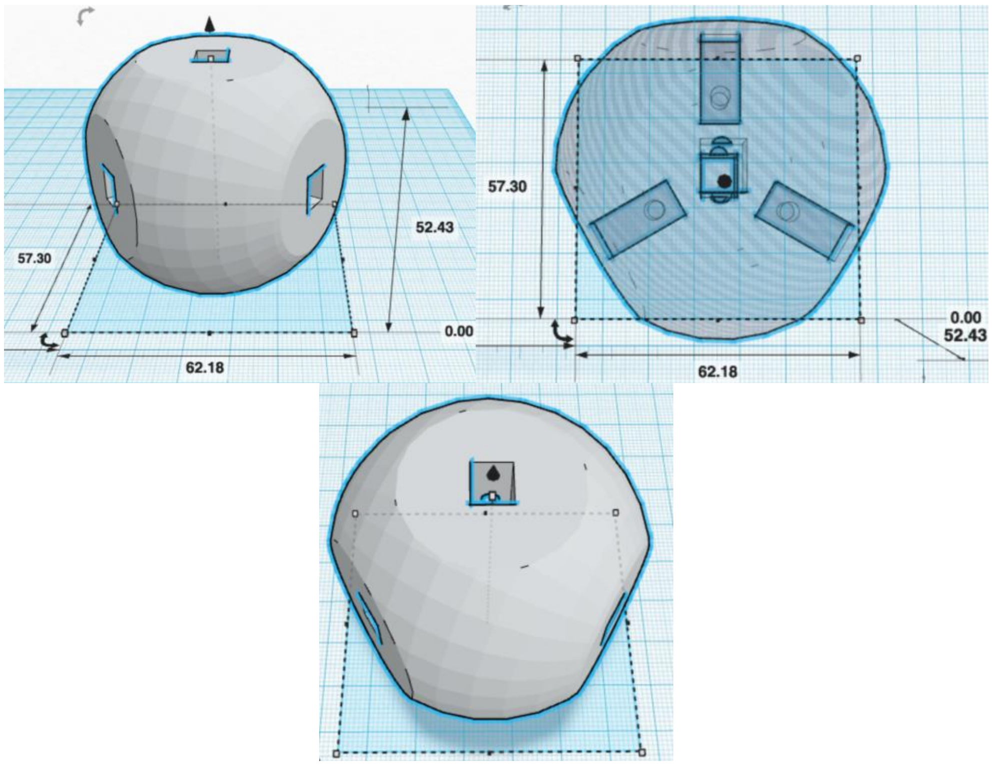
The pi bond was designed using a lone pair/ orbital as the starting point. The distance between two printed sp^2 atoms connected by a bond was measured, transferred to Tinkercad and two lone pairs were placed at this set distance. These were then each trimmed to provide a flat surface with which to develop a pi bond 'bridge' between the two. Once complete, the design was duplicated, clips added for subtraction and the lone pairs deleted to leave the bridge as a single printable object.



Supplementary Figure 15. Model of pi bond bridge and connecting orbitals.

2p orbital for pi bond		**Pi bond 'bridge'**	
Infill Percentage:	10%	**Infill Percentage:**	10%
Material:	ABS/ PLA	**Material:**	ABS/ PLA
Total Weight:	36.94 g	**Total Weight:**	18.65 g
Cost estimate:	$ 0.97	**Cost estimate:**	$ 0.49

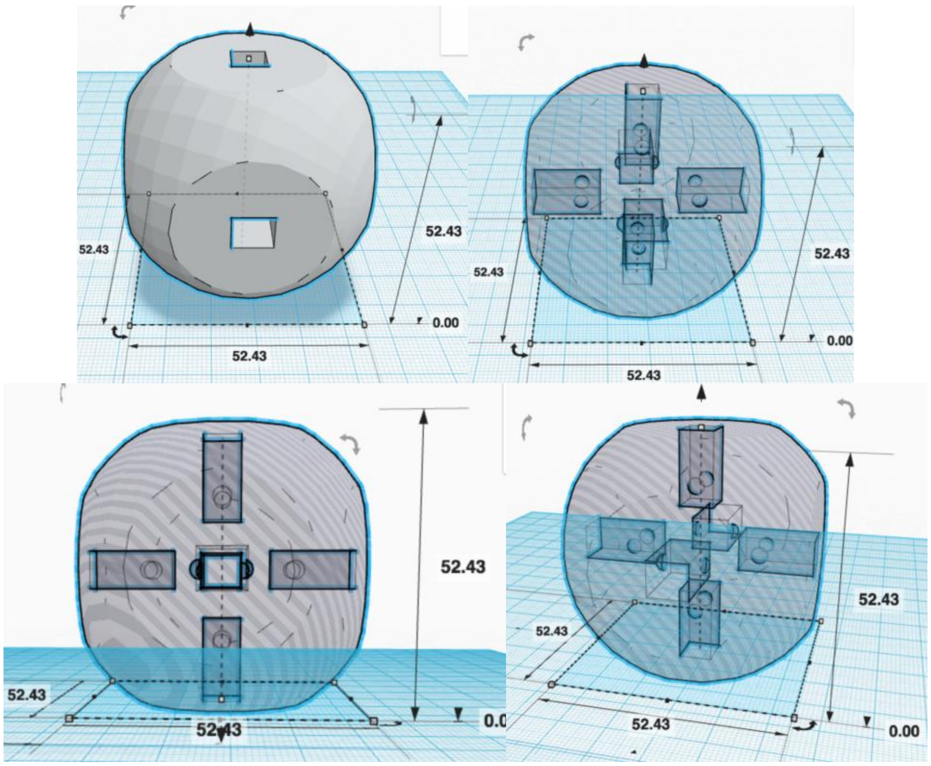
sp^2 carbon atom with pi bond/ 2p orbital attachment



210 **Supplementary Figure 16**. Model of sp^2 atom with pi bond/ 2p orbital attachment point.

Infill Percentage:	10%
Material:	ABS/ PLA
215 **Total Weight:**	20.70 g
Cost estimate:	$ 0.55

sp carbon atom with two pi bond/ 2p orbital attachment points



Supplementary Figure 17. Model of sp atom with two pi bond/ 2p orbital attachment points.

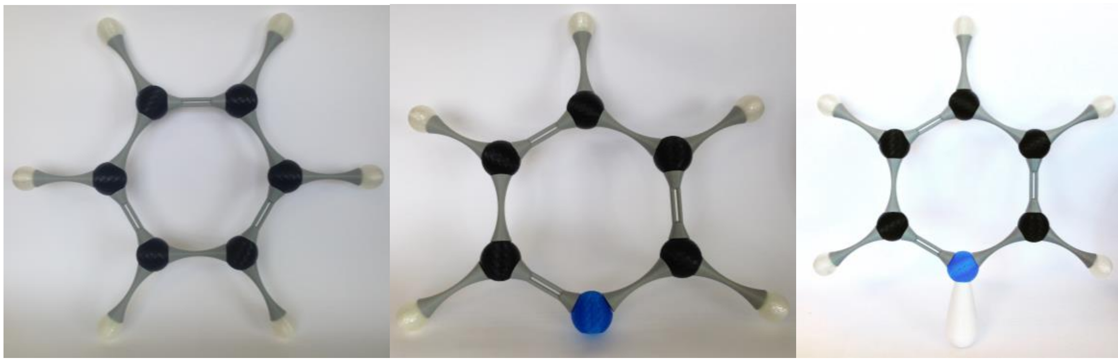
Infill Percentage: 10%

Material: ABS/ PLA

Total Weight: 20.27 g

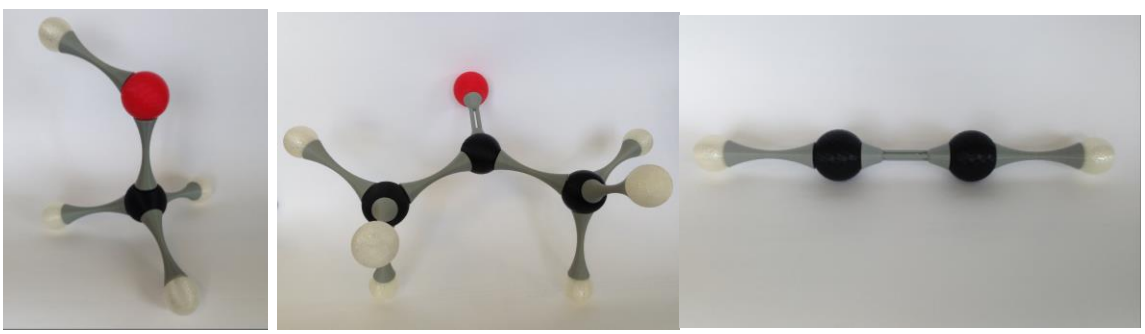
Cost estimate: $ 0.53

Lecture-size models of benzene and pyridine



Supplementary Figure 18. Large scale models of benzene (left) and pyridine (center) with the lone pair on the right hand model clearly highlighting its location within the plane of the ring and hence, availability for protonation (right).

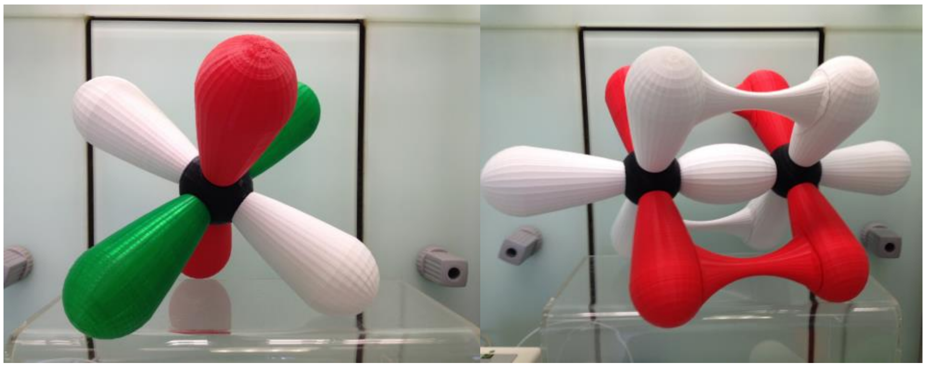
Lecture-size models of methanol, acetone and acetylene



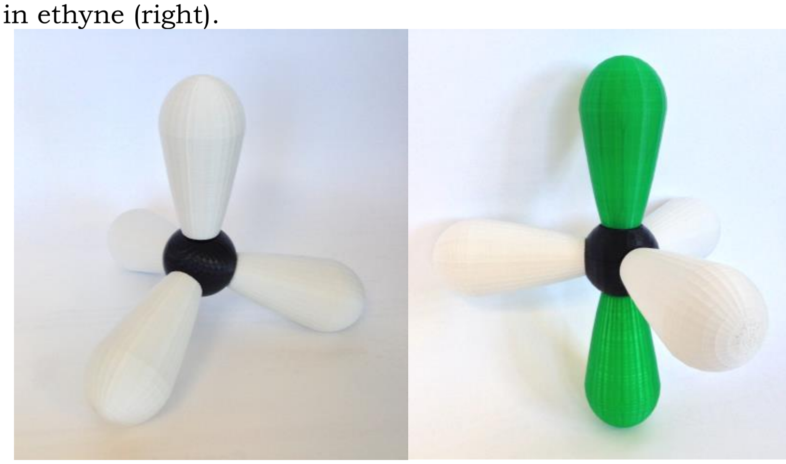
Supplementary Figure 19. Large scale models of methanol (left), acetone (center) and acetylene (right).

Lecture-size orbital models

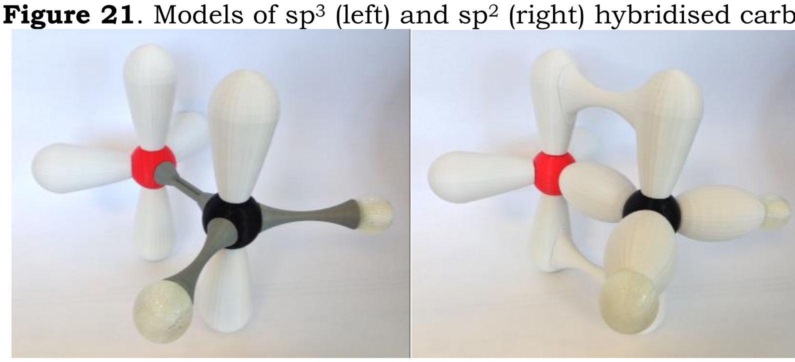
Using the orbital models in a range of colours, a number of concepts can be easily represented for students ranging from ready display of p-orbitals through to hybridisation and bond rigidity (Supplementary Figure 20-22).



Supplementary Figure 20. Models of an sp hybridized carbon atom (left) and molecular bonding orbitals in ethyne (right).

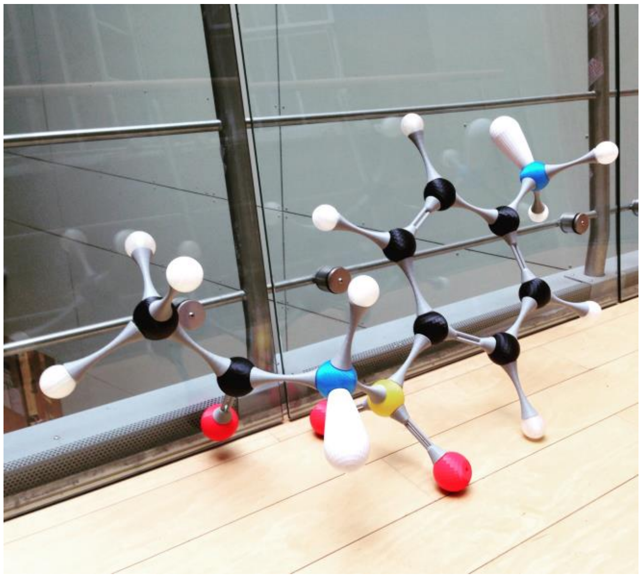


Supplementary Figure 21. Models of sp^3 (left) and sp^2 (right) hybridised carbon atoms.

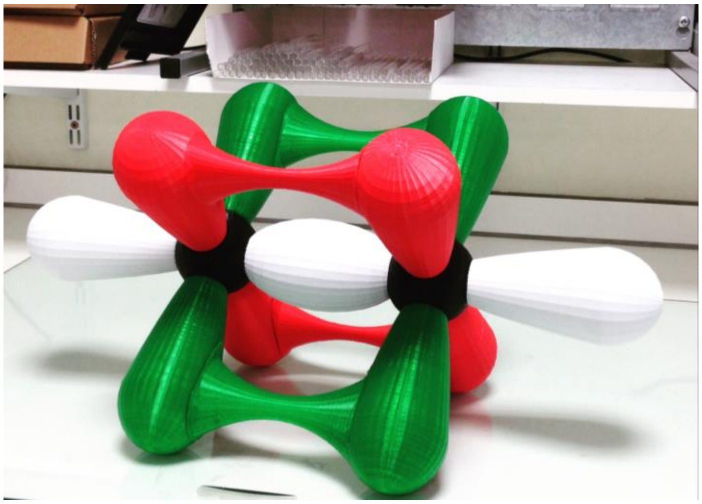


Supplementary Figure 22. Models of formaldehyde with (left) and without (right) pi bond bridge.

Large-scale model of sulfacetamide and an orbital model of acetylene



Supplementary Figure 23. Large scale model of sulfacetamide highlighting the size of the printed models.



Supplementary Figure 24. Large scale orbital model of acetylene highlighting the size of the printed model.

Workshop-scale (50%) models

The models prepared for the lecture based series were remodeled and scaled at 50% in order to develop workshop applicable models. One of the benefits of this approach is that multiple models can be built in a single print. Examples of these are shown in the following pictures. Models were printed on MakerBot mini printers and as can be seen below (Supplementary Figure 19) up to 20 bonds can be printed in a single print run. All models were printed at 10% infill (except bonds at 40%), with no support and 2 layers.

Supplementary Figure 25. Illustration of the numbers and types of prints that can be carried out using this approach. In the middle figure, mixed orbitals can easily be printed.

Supplementary Figure 26. Illustration of the multiple print options on each print bed.

Supplementary Figure 27. Model of cyclohexane on the bed of a MakerBot printer highlighting the size of the finished model.