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Technology Report

Visualizing 3D Molecular Structures Using an Augmented Reality App

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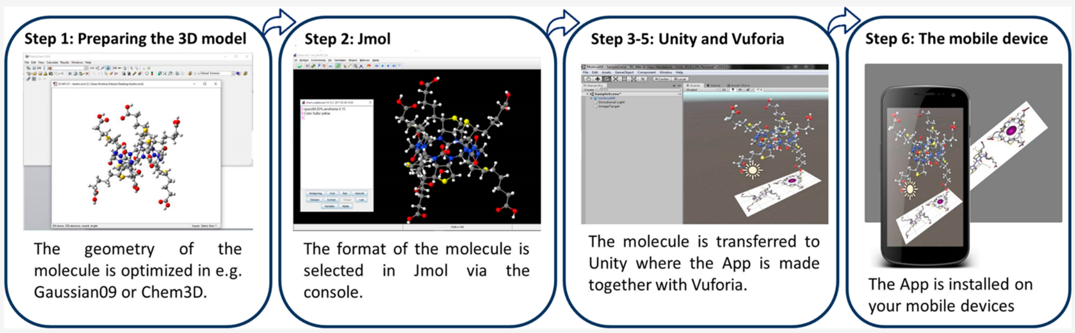

ABSTRACT: We present a simple procedure to make an augmented reality app to visualize any chemical 3D model. The molecular structure may be based on crystallographic data or from computational modeling. This guide is made in such a way that no programming skills are needed, and the procedure uses free software and provides a way to visualize 3D structures that are normally difficult to comprehend in the 2D space of paper. The process can be applied to make a 3D representation of any 2D object, and we envisage the app to be useful when visualizing simple stereochemical problems, when presenting a complex 3D structure on a poster presentation or even in audio-visual presentations. The method works for all molecules including small molecules, supramolecular structures, MOFs, and biomacromolecules.

KEYWORDS: *Computer-Based Learning, General Public, First-Year Undergraduate/General, High School/Introductory Chemistry, Elementary/Middle School Science*

■ INTRODUCTION

Conveying information about three-dimensional (3D) structures in two-dimensional (2D) space, such as on paper or a screen, can be difficult.[1] Augmented reality (AR) provides an opportunity to visualize 2D structures in 3D, and AR has transformed visualization in computer games and films, but the technique is distinctly underused in (chemical) science.[2−4] AR is a fairly new technology, but its popularity is increasing quickly; chemists are slowly starting to explore the benefits of using AR in teaching.[5,6] Studies examining the potential of using AR apps (applications) as a tool in teaching chemical problems have yielded promising results.[7,8] However, only a few AR apps trying to support students in learning and understanding chemical problems are available.[9−11] Furthermore, these apps have until now been limited to visualizing specific molecules or teaching exercises.[9−11] Fortunately, software to make simple AR apps is becoming common, and ranges of free software now exist to make customized apps.[12] This opens the opportunity for a chemist with no programming experience to create their own AR app and include their own molecules of interest. In chemical science, the challenge of visualizing in 3D exists at several levels ranging from teaching stereochemistry problems at the freshman university level to visualizing complex molecular structures at the forefront of chemical research. Visualization can be especially challenging since molecules are getting larger and more complex and span three dimensions. An elegant way to visualize molecules in 3D is to 3D print the desired structure, and protocols of how to do this starting from molecular structures have recently been described.[13] To describe the geometry and symmetry of complex molecules, chemists are often forced to draw molecules in simplified or schematic ways and thus neglect information. One example of a highly complex molecule that is difficult to display in 2D is the molecular Borromean rings molecule prepared by Stoddart and coworkers (Figure 1a). In their structural representation, some atoms and labeling of atoms are omitted to simplify the structure.[14] In the simplified 2D image, bonds and atoms are

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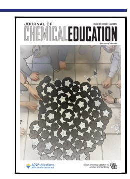

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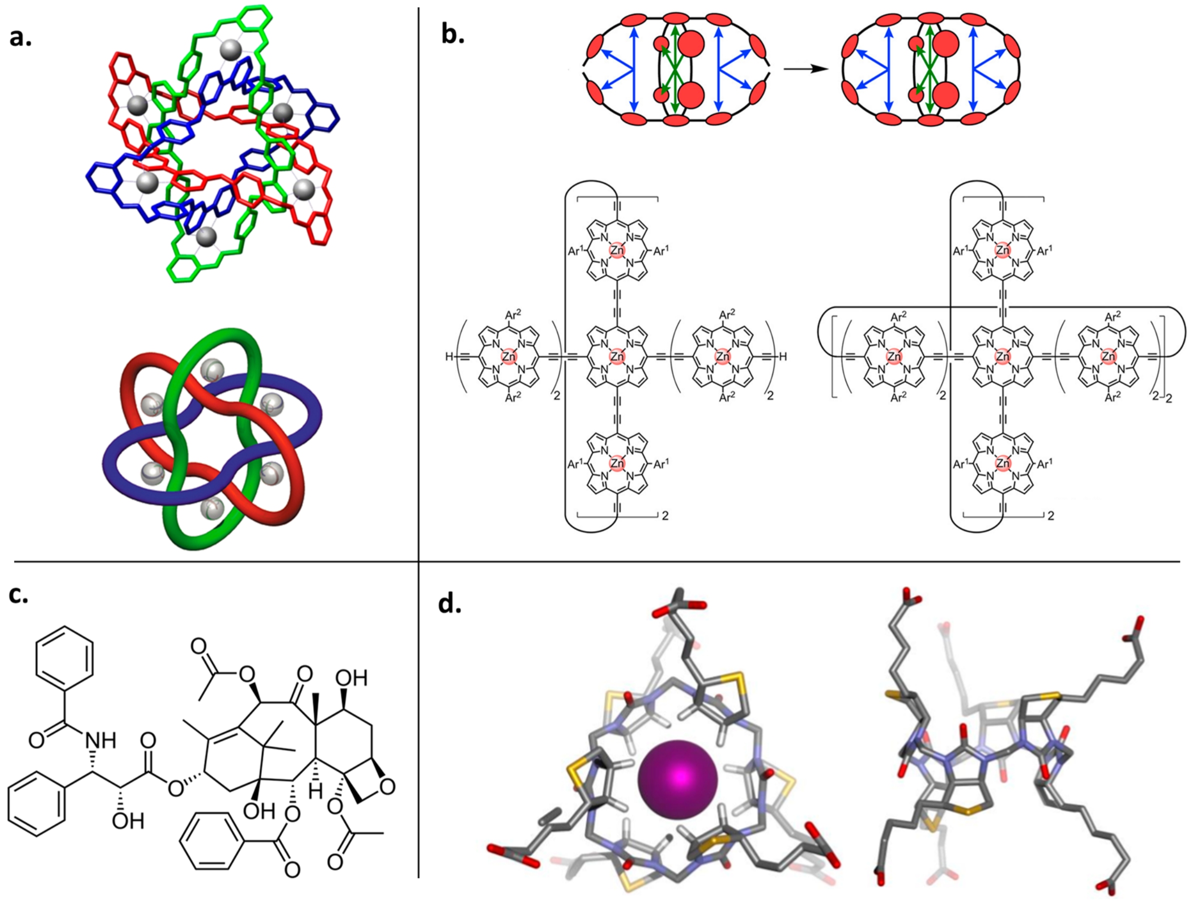

Figure 1. Examples of complex molecules that are difficult to comprehend in 2D. Download the AR app on a device (phone or tablet) to view these structures in AR. The app can be found via the QR code or the link in Figure 2. (a) The Borromean rings are shown two different ways to emphasize the geometry and symmetry of it. (b) The porphyrin nanoball is presented two different ways to highlight the geometry and the connection of the different elements in the nanoball. (c) Paclitaxel is a complex molecule with many stereocenters. A 3D view of it helps to appreciate the complexity and may aid retrosynthetic analysis. (d) A top view and side view of the crystal structure of the biotin[6]uril. Download the app by following the link in Figure 2, and see how the AR works.

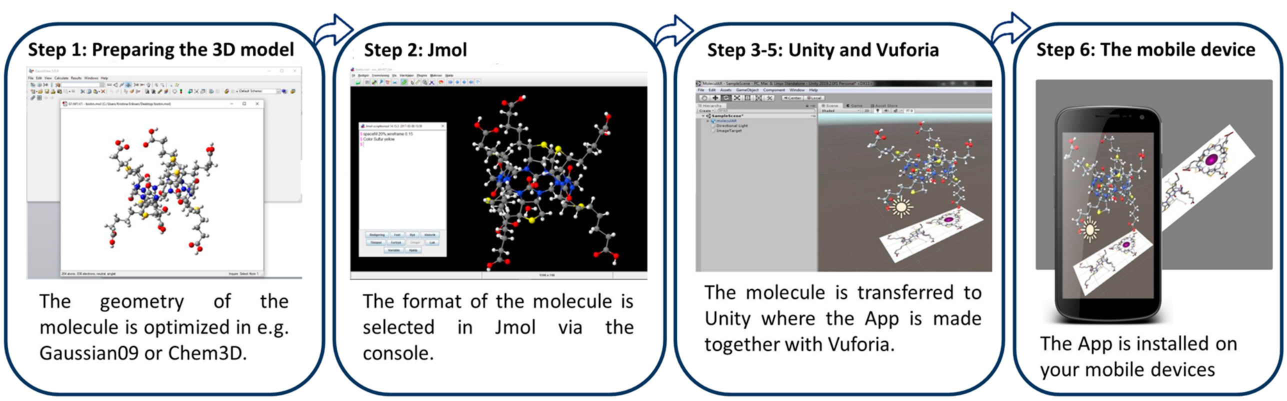

Figure 2. Work flow for making AR apps using free software. Link to the AR app: https://play.google.com/store/apps/details?id=com.UniCPH.Android.MoleculAR.

overlapping and thus still make it difficult to visualize the geometry and symmetry. Many chemists even draw the same molecule twice in different formats in the same paper to better explain the connections of the different elements and its geometry. This is illustrated with the porphyrin nanoball by Anderson (Figure 1b) and the supramolecular complex between biotin[6]uril and the iodide anion (Figure 1d).[15,16] It can be challenging to come up with a new synthetic route for complicated molecules such as paclitaxel (Figure 1c), because it is hard to visualize how sterically congested regions affect each other.[17] For these types of problems described above, a simple way to visualize molecules in 3D would be beneficial.

■ WORK FLOW

In this contribution we describe how to make a simple AR app for a mobile device (e.g., phones and tablets) to visualize

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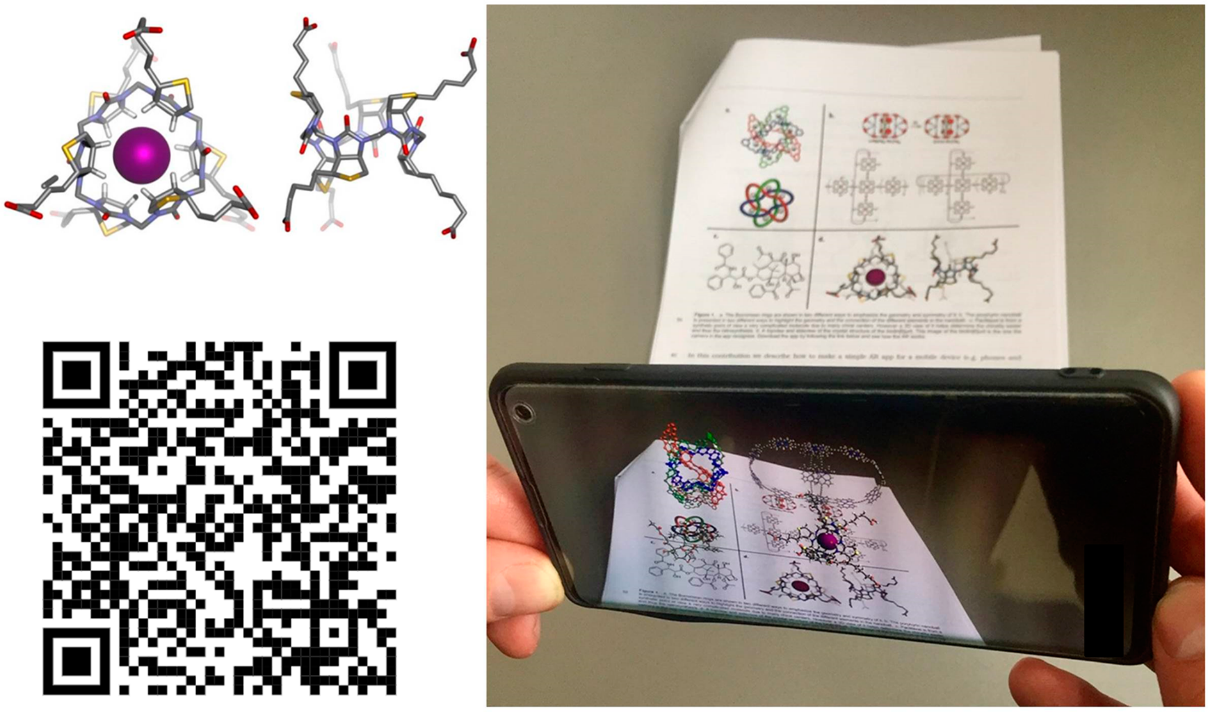

Figure 3. A 2D image of Biotin[6]uril. Download the app from the link below or the QR code and point the mobile device to see the structure in 3D through the camera. https://play.google.com/store/apps/details?id=com.UniCPH.Android.MoleculAR.

molecules in 3D. It is important to emphasize that this guide is made in such a way that no programming skills are needed, and that only free software is used. The work flow is rather simple (Figure 2): First, a molecular model is generated from molecular modeling, from a single crystal X-ray structure or similar. The model is taken through a series of easily downloadable free pieces of software (Jmol, Unity, and Vuforia) to give the custom AR app. The first time, this process of making an AR app takes ca. 2 h to download all the software and familiarize the user with the software. A thorough point-by-point guide of how to make custom-made AR apps is given in the Supporting Information. Subsequent AR apps are then much simpler to generate and take only a few minutes.

The procedure for preparing the AR app was optimized by 6 members of a university research group, and the premade app (download via QR code, Figure 3) was tested by a Danish high school class (24 students). This verifies the applicability of the point-by-point guide to how to make custom-made AR apps (Supporting Information). The prepared apps were used by the students on poster presentations and in reports.

While all software is easily available, it does from time to time cause difficulty for some users with preparing their own app using the guide (SI) in the first attempt. If this tool is to be used in a teaching situation, it is important that the teacher spends a few hours learning to use the different software items, in order to effectively guide students toward success preparing their own apps. This was also pointed out by the reviewers of this paper, and to effectively use this tool in a teaching situation, it is advised that groups of students work together to effectively can help each other.

When the app is made, it is free to transfer the app via a USB cable from the computer to the mobile devices. However, publication of the app in Google Play requires a one-time payment to Google Play of $25 (2020).

When the AR app is made and transferred to a mobile device, a camera opens, and it recognizes a chosen image. The image may be on a poster, in a book, or on a screen. The recognition leads to a 3D model (of one or more molecules of the user's choice) opening as a part of the real world through a mobile device. When all the software is installed correctly, the app is simple to make and can be used at a poster session or in the classroom. One can download an example of the AR app (follow the link or QR code above) on an Android mobile device and see how it works and what it looks like (in the real augmented world). Once the app is downloaded and opened, one can then point the camera at Figures 1 and 3, and a 3D model of the molecules will appear.

■ CONCLUSION

We have described how to make a simple augmented reality app to visualize any 3D chemical model using free software. The method works for all molecules including small molecules, supramolecular structures, MOFs, and biomacromolecules.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.9b01033.

Directions for creating a molecular model and developing relevant software (PDF, DOCX)

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Notes

The authors declare no competing financial interest.

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