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# Visually impaired researchers get their hands on quantum chemistry: application to a computational study on the isomerization of a sterol

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**Abstract** In molecular sciences, articles tend to revolve around 2D representations of 3D molecules, and sighted scientists often resort to 3D virtual reality software to study these molecules in detail. Blind and visually impaired (BVI) molecular scientists have access to a series of audio devices that can help them read the text in articles and work with computers. Reading articles published in this journal, though, is nearly impossible for them because they need to generate mental 3D images of molecules, but the article-reading software cannot do that for them. We have previously designed AsteriX, a web server that fully automatically decomposes articles, detects 2D plots of low molecular weight molecules, removes meta data and annotations from these plots, and converts them into 3D atomic coordinates. AsteriX–BVI goes one step further and converts the 3D representation into a 3D printable, haptic-enhanced format that includes Braille annotations. These Braille-annotated physical 3D models allow BVI scientists to generate a complete mental model of the molecule. AsteriX–BVI uses Molden to convert the meta data of quantum chemistry experiments into BVI friendly formats so that the entire line of scientific information that sighted people take for granted—from published articles, via printed results of computational chemistry experiments, to 3D models—is now available to BVI scientists too. The possibilities offered by AsteriX–BVI are illustrated by a project on the isomerization of a sterol, executed by the blind co-author of this article (HBW).

**Keywords** Molecular 3D-print · BVI scientists · 2D to 3D

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## Introduction

Pondering structures of molecules has always been intimately connected to their visualisation. Indeed, in the middle of the nineteenth century, long before anything was known about the physical structure of atoms and the exact way they combine to form molecules, scientists such as Kekulé had already made 3D molecular models using the balls of the boring game of croquet [1]. Today, one is hard pressed to find an article in this journal that does not show at least one visual representation of a molecule. The necessity in chemical research to visualise molecules creates a tremendous hurdle for blind and visually impaired

(BVI) scientists. Assistive tools must be developed in the field of chemistry to allow BVI scientists to access the full wealth of molecular information in articles in this journal and to benefit from equal access to higher education in science. It is the experience of the blind co-author of this article (HBW) that once a chemical structure is in his mind, he can hold on to that image and think about associated chemical concepts with little trouble.

BVI individuals use Job Access with Speech (JAWS) or other text-to-speech software to read information displayed on a computer screen (e.g., webpages and electronic books), live readers and such software to read figure-heavy articles, and a combination of 2D figures created by live readers and tactile relief prints created with a Pictures in a Flash (PIAF) machine to gain access to 2D images [2–5]. Tools that can aid a BVI scientist with the generation of 3D images of a molecular structure, however, are not routinely available yet. The concept of using 3D printing to make chemistry more accessible to the blind is not new. 3D printing was, in fact, employed by Skawinski and others as early as 1995 for making molecular structures tactilely accessible. This method, however, did not use a computer-generated model and employed a primitive 3D printer [6–8].

While relief printers can convert 2D images into relief plots that can be felt by BVI scientists, feeling the structures of organic molecules such as inhibitors for enzymes, ligands for receptors, etc., is still difficult because pictures of molecules are rarely produced with BVI scientists in mind. Details that may be considered insignificant to sighted people may render molecular images unreadable for BVI individuals. For instance, the structure of some complex organic molecules can be represented in 2D by having bonds cross over one another with the bond furthest from the viewer 'broken'. This drawing convention is inaccessible to BVI chemists because the broken bond lines at these crossings often feel like unlabelled vertices. 3D models, however, present the connectivity of atoms in a model in a completely unambiguous manner. Thus, we turned the focus of our work to creating annotated 3D models both of molecular structures in PDF files and molecular structures investigated computationally by HBW who is a PhD student in chemistry.

Sighted chemists routinely deal with 2D and 3D chemical models. Most low molecular weight compounds exist as 2D models stored in electronic databases or as 2D sketches published in documents such as articles or patents. AsteriX [9] is an interactive website that reads these types of documents in PDF format. It detects 2D plots of low molecular weight molecules, removes meta data and annotations from these plots, and converts them into 3D structures that can be visualized in many ways either via the website or using in-house visualisation tools. Most visualisation tools give sighted researchers a good sense of three-dimensionality, but to BVI individuals these representations remain as 'flat' as the screen of their computers. A Google-image search for "3D print molecule" results in thousands of hits of beautifully produced 3D models, but almost none of these are of any use for BVI scientists because, for example, most of them are too small, and CPK colouring of atom types does not add anything to their experience.

We have modified AsteriX to provide an assistive interface for BVI researchers and to create tactile models that can be 3D-printed in plastico. We integrated the widely used Molden package [10] in AsteriX, which enabled the materialisation of quantum chemistry calculations performed with ab initio and density functional theory (GAUSSIAN, GAMESS-UK, GAMESS-US) and Semi-Empirical (Mopac/Ampac) software packages using a newly developed CAD program that converts AsteriX results into files containing printable tactile 3D models. In addition, we developed software that converts X–Y plots into Braille plots with Braille annotation, and we modified AsteriX' project management tools to be better suited for BVI scientists.

We demonstrate the capacities of AsteriX–BVI with a project in which HBW investigated the mechanism of a carbocation rearrangement of a naturally occurring sterol. This sterol contains 30 carbon atoms and is structurally complex, thereby providing a meaningful test of AsteriX–BVI.

We believe AsteriX has the potential to become an assistive website broadly employed by BVI students in the coming years. For example, AsteriX–BVI can already produce tactile 3D models in which the types of atoms are indicated both using colours and atom types with specific haptic (tactile) characteristics. We believe that application of such options would help to put BVI and sighted researchers on an even playing field with respect to molecular visualisation.

## The AsteriX 2D-to-3D molecular image converter

AsteriX is a publically available website and web server that was originally designed to automatically extract chemical structures represented in schematic drawings as 2D sketches. AsteriX automatically extracts images from PDF articles and analyses them to determine whether they contain representations of small organic molecules. Areas in an image that are identified as potentially containing organic molecules are subsequently analysed in terms of atom types, connectivity, bond types, and stereochemistry. This allows for the spatial reconstruction of the ligand topology and the subsequent generation of a 3D model via 2D-to-3D conversion using molconverter from ChemAxon [11]. The flow scheme of AsteriX is depicted in Fig. 1.

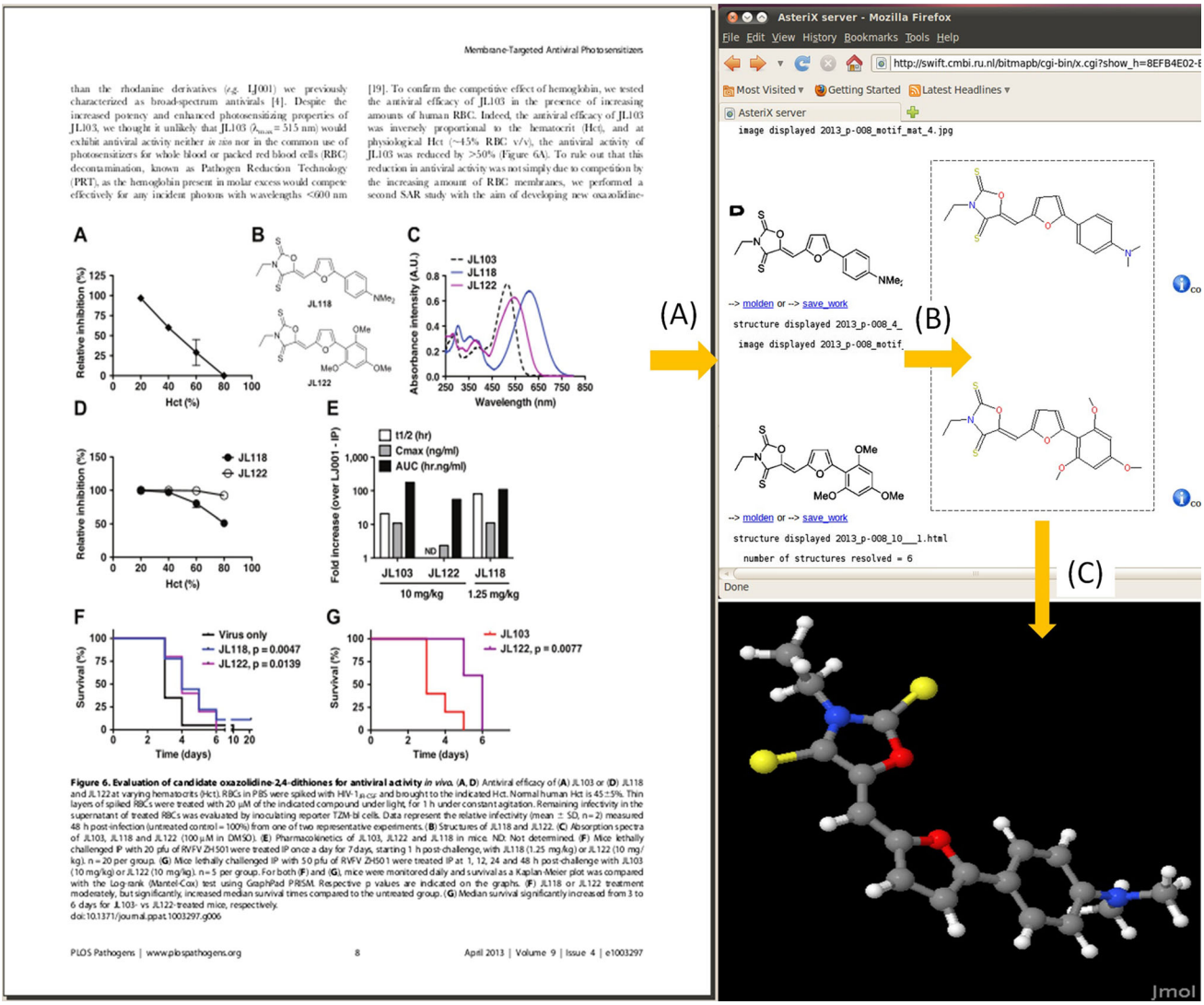


**Fig. 1** Flow scheme of AsteriX. **a** AsteriX automatically detects pictures in PDFs that contain 2D molecules [12]. **b** It removes non-molecular aspects such as annotations, graphs, bar diagrams, etc., and decomposes the remaining parts of the picture into individual molecules (assessing atom types, bond orders, and connectivity). **c** It then makes a 3D representation that, for example, can be visualized at the website as a sphere-and-rod model

AsteriX' potential to assist BVI chemists was recognized by the blind co-author of this article (HBW), who is pursuing a PhD degree in chemistry at the University of California—Davis. His realisation triggered the upgrade from AsteriX to AsteriX–BVI.

When a BVI scientist uploads a PDF file containing 2D molecular images, a large series of consecutive steps gets triggered. First, AsteriX converts 2D representations of molecules into 3D structures as described before [9] (see Fig. 1). The extension of AsteriX to AsteriX–BVI required a series of steps. First, the website needed minor modifications to enable BVI scientists to use it through JAWS [2], the assistive software that reads aloud the contents of websites and helps BVI users with the website navigation. After these modifications were completed, two major additions were implemented: 3D printing of molecules, and Braille printing of plots, annotations, and meta data.

AsteriX–BVI has to execute a series of steps to arrive at a 3D-printable version of a molecule. Atom types need to be made recognizable by surface haptic elements, and bonds marked by different polygonal cross sections with haptic characteristics, including Braille meta data text on those bonds. For BVI scientists there is a practical lower limit (in terms of readability with one's hands) of about 3.5 cm on bond lengths. This may result in the necessity of having physical 3D models bigger than the print volume of today's printers so that it becomes essential to split 3D molecules into fragments that can be printed separately and then easily and unambiguously be assembled.

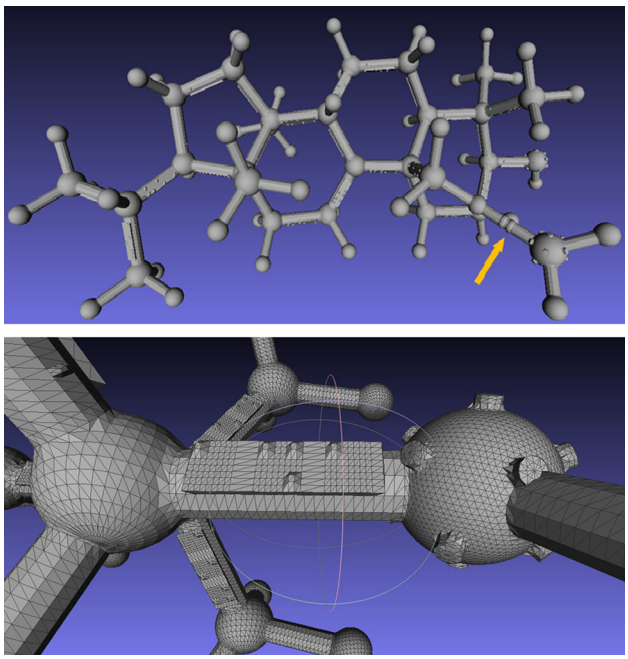

**Fig. 2** Example of a haptic (tactile) model calculated by AsteriX-BVI. Particular geometries are used instead of colours to represent different types of atoms and bonds. For instance, carbon atoms are simple spheres while an oxygen atom is represented by a sphere covered with small cylinders. *Top* overview. *Bottom* bond length, an important parameter in quantum chemistry, is embossed in Braille on a bond in the model. The *bottom plot* makes clear why a triangular mesh of no <140,000 tiles was needed for this 3D model. Water molecules that may intervene in quantum calculations (*top view*) are connected to the structure via a special type of tactile bond (*orange arrow*, see also Fig. 6; "Bond types" section)

## AsteriX–BVI methods and implementation

Use of AsteriX by sighted people is rather straightforward, but BVI scientists need a project space on the server to perform all manipulations easily. The 3D coordinates need to be converted to the stereolithographic format (.stl) by our specialized CAD program, which needs to deal with the haptic elements for bond types and atom types and should intelligently split molecules that are too large for the build volume of a given 3D printer. The software must be able to produce Braille annotation both on the actual 3D model and in meta data files. Figure 2 shows an overview of a molecular model to be printed in 3D, and illustrates some of the haptic details.

After interpreting a 2D image of a molecule, AsteriX produces a 3D sdf file that contains information about covalent bond types (single, double, triple, and aromatic). However, when AsteriX deals with the result of quantum calculation, water molecules may be positioned around the studied small molecule to intervene in QC calculations. It was thus of importance that those waters in close contact remain physically linked to the printed 3D model. Intermolecular hydrogen-bonds are determined for these waters by a program subroutine that only uses geometrical considerations. Intermolecular hydrogen bonds must, of course, be printed as solid bonds so that the relationship between the hydrogen bonded molecules is not lost the moment the molecules are removed from the build volume of the printer (see Fig. 2).

3D printers require a triangular mesh defining the outer envelope of the print model in .stl format. To produce the triangular meshes defining such an envelope surface we have written a computer aided design (CAD) code (Fig. 3) that use cylindrical (r, θ) coordinates to generate bonds. When printing 'normal' 3D molecules one would use a large number of θ increments to obtain smooth, round bonds. We deliberately use small increments to produce atomic bond cross-sections of various polygonal shapes: dodecagons, hexagons, and squares to represent single, double and triple bonds, respectively (Fig. 6). Atoms need haptic elements to allow the difference between atom types to be felt. The absence of haptic elements also is a haptic characteristic, so we decided to produce smooth surfaces for the most common atoms carbon and hydrogen. The latter is the much smaller and thus also easy to recognize without haptic elements. These atoms are produced using spherical (r, θ, φ) coordinates. All other atom types are produced using a dedicated method.

### Atom types

To identify different atom types we established a minimal set of simple geometries defining haptic characteristics that can be easily recognized by the fingers. To define atom types we used smooth spheres for C and H, and spheres covered with small structural elements: pure icosahedrons, icosahedrons covered with small cylinders positioned at the vertices or centred on facets, and icosahedrons covered with small half-spheres centred on facets. In addition, a scaling factor is ascribed to every atom. It allows the radii of the associated haptic sphere or icosahedron to be scaled according to the type of chemical element it represents. We thus produced seven distinct geometries, the size of which can be incrementally tuned from small (0.9 cm diameter), to medium (1.2 cm), large (1.5 cm), and very large (1.8 cm) to allow for more atom types. The combination of atom surfaces and atom radii allows us to define 19 distinct haptic atom types (Fig. 4) that we use to describe the chemical elements most relevant for organic chemistry. Entire categories and groups of elements in Mendeleev's periodic table, for instance transition metals, lanthanides and actinides, may all be represented by the same atom type, provided that structure annotations in connection with the model and provided on the server or on a small printable label, that can be attached to the model (Fig. 5)

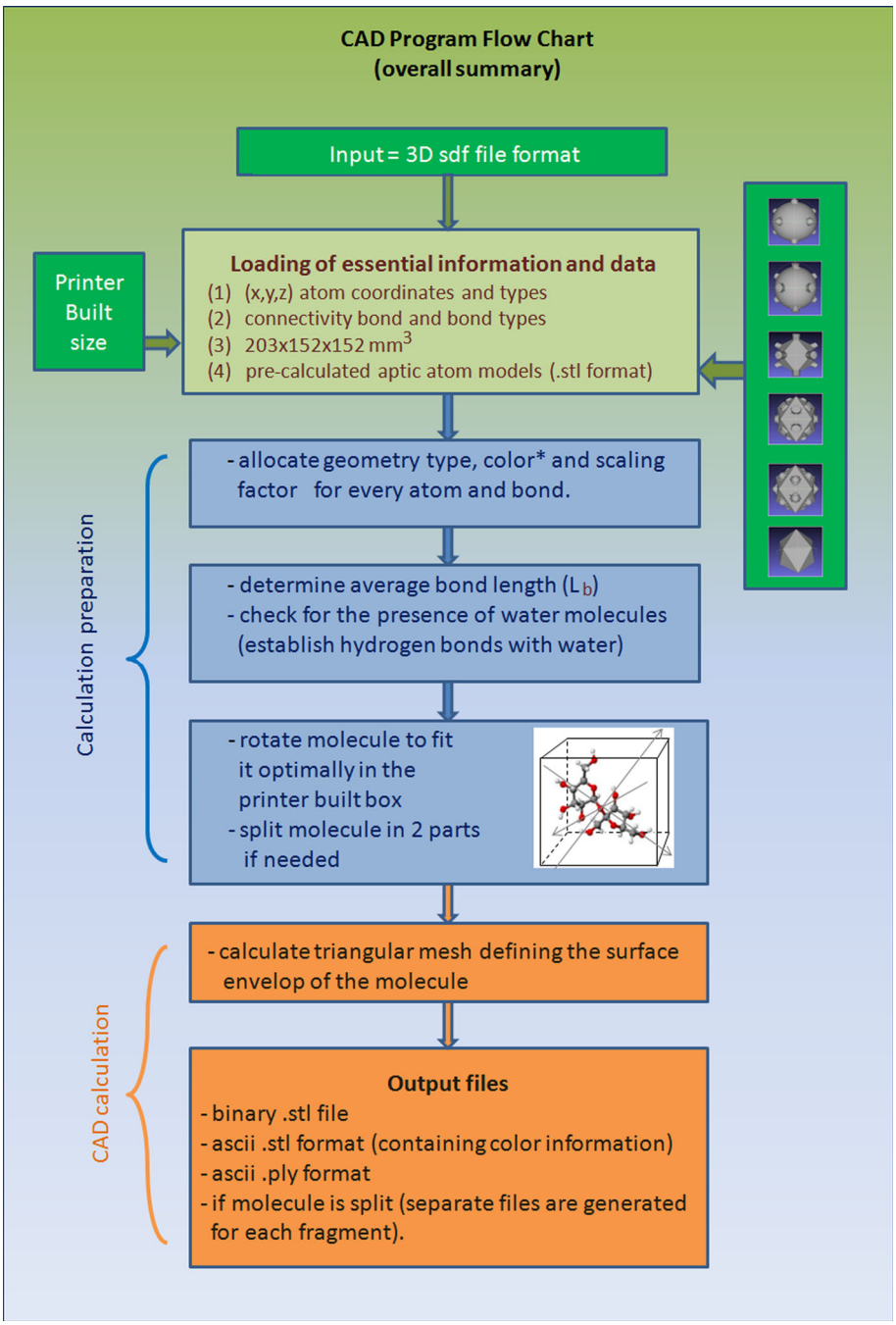


**Fig. 3** Flow chart for the CAD program. In the first stage of its execution (*green area* in the flow chart), the program reads the molecule to be converted into a haptic model as a 3D .sdf file that contains all information needed to reconstruct the molecule's chemical structure (atom types, bond types, connectivity). The pre-calculated haptic atom types must be provided in ASCII .stl format. Additionally, the program needs to know the printer build volume dimensions. The next stage (*blue area*) consists of: allocating haptic geometries and colour to every atoms and bond, determining the average bond length ($L_b$) between non-hydrogen atoms and check for the presence of water molecules and the possible presence of intermolecular hydrogen bonds. Then, the molecule is oriented inside the build volume to optimize the size of the printed model. Using $L_b$ and the build sizes in the X, Y, Z directions it is determined whether the molecule must be split or not in order to print a model with bond length of ca. 3.5 cm (between non-hydrogen atoms). Finally, the haptic surface envelop of the molecule is calculated (*orange area*) and printed in three different formats (binary .stl; ascii .stl; .ply). When splitting is needed two sets of files corresponding to the two halves of the molecule are generated. *Anticipating the possibility that 3D printers will routinely produce coloured models in the coming years, CPK colours are ascribed to atom types

explain which atom types are meant (we have only a label with the name of the project on it at this moment).

We have used spheres and icosahedrons generated with MeshLab, a publically available CAD program [13] to generate the non-smooth special atom types as starting material. The regular surface tessellation of the basic spheres and icosahedrons produced by MeshLab were made of 5,112 and 1,308 triangular tiles, respectively. We used these basic geometries to generate, with our own codes, more complex surface envelopes to create atom types with specific haptic properties (Fig. 4). Surface tessellations of haptic atom types are stored as input files for our CAD code and thus do not need to be recomputed for every atom and every structure, thus improving computational efficacy. Figure 5 shows an example of the use of special atom types.

## Bond types

Cylinders with dodecahedral, hexagonal, and square cross-sections were chosen to represent single, double and triple bonds, respectively (Fig. 6). Besides the geometrical shape

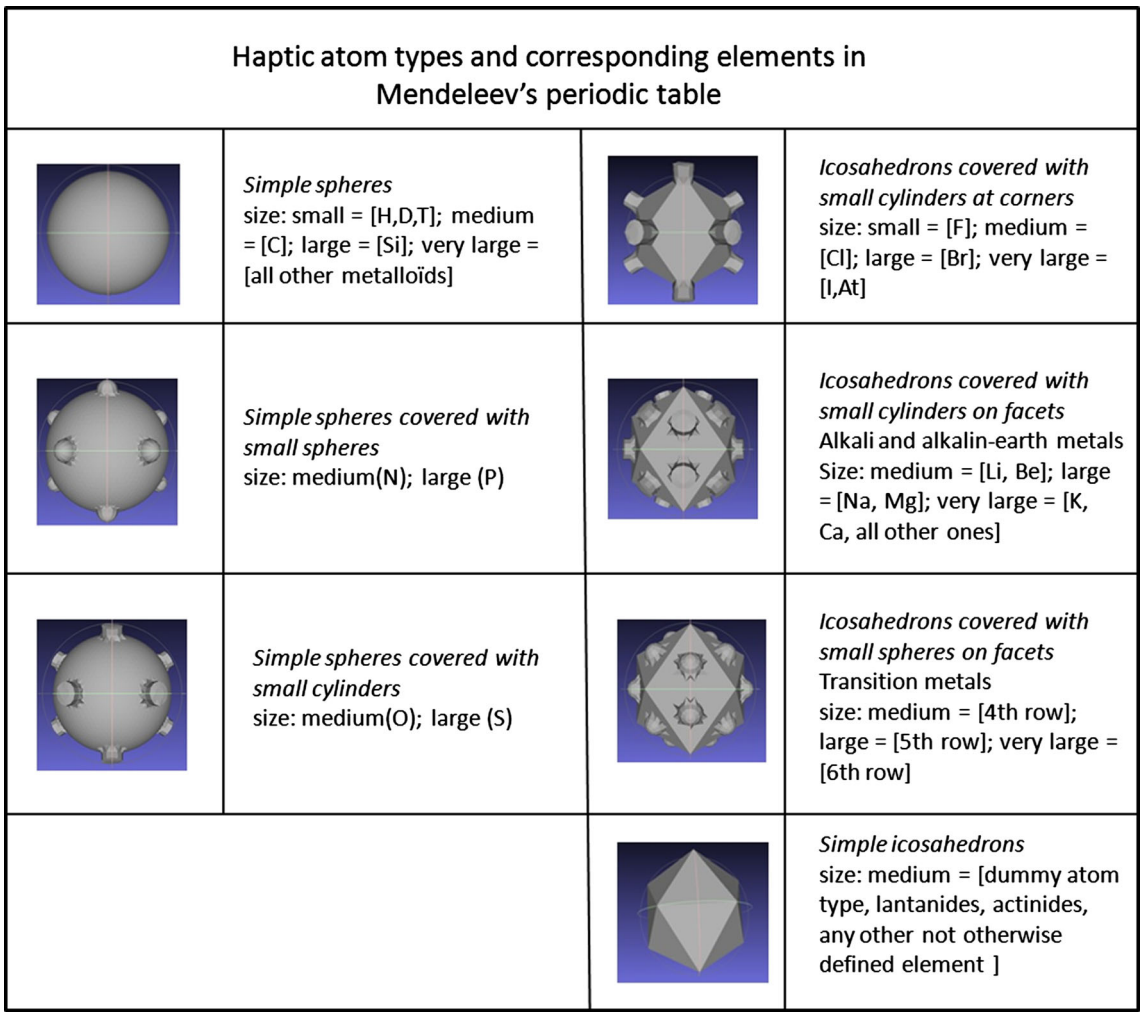


**Fig. 4** Seven different spheres and icosahedrons with various surface characteristics and radii that define haptic (tactile) atom types BVI users can recognized with their fingers. This set of geometrical shapes allows for the creation of 19 haptic types of atom, a number sufficient to effectively deal with the construction of adequate models for most organic molecules and organometal complexes

of their cross sections, additional haptic characteristics are used to differentiate bonds. To generate three additional bond types (aromatic; half-bonds; non-covalent bonds/hydrogen bonds) we use dodecagonal cylinders with carved or protruding notches in the middle (Fig. 6). This way we can produce six different bond types. We point out that, that hydrogen-bonds are materialized by a cylinder that actually connects the hydrogen of the H-bond donating group to the acceptor atom instead of connecting the two electronegative atoms. A small protruding pane is generated at the surface of each bond between non-hydrogen atoms on which bond length calculated from the x, y, z coordinates of atoms in the sdf file is indicated in Braille in units of 0.01 Å.

## Surface tiling

Present day 3D printers require that the surface mesh presented in the .stl file is absolutely perfectly closed. The 3D printer software is still a bit unforgiving, as demonstrated in Fig. 7b where the result of a 3D print in which just a few of the more than a hundred thousand surface tiles were missing.

Obtaining a continuous mesh of triangular tiles that accurately covers the surface envelope at the locations where atom spheres (and icosahedrons) and bond cylinders intersect was the main difficulty encountered in designing the CAD program. Figure 7a illustrates some of the problems that had to be solved.

## Molecule splitting

We empirically determined that bonds can be easily recognized by fingers when the length of printed bonds between two non-hydrogen atoms is approximately 3.5 cm, atom centre to atom centre. Bonds should be approximately 0.7 cm thick. Atom diameters are optimal around 1.3 cm

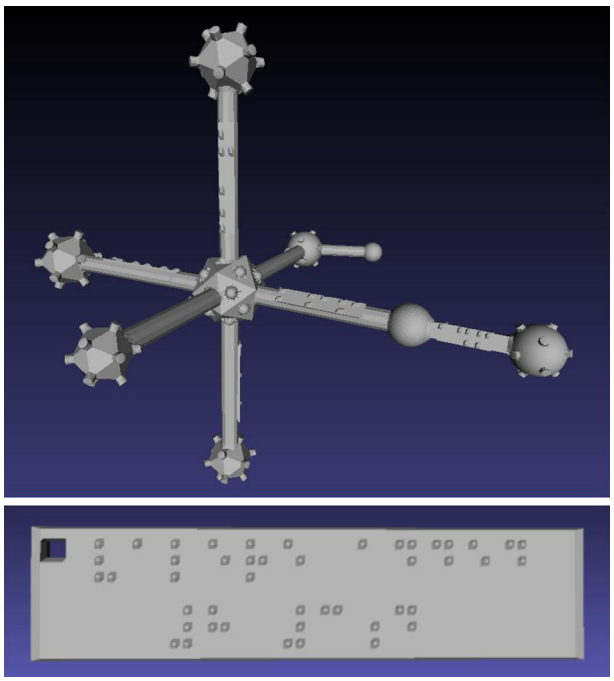

**Fig. 5** Example of haptic (tactile) model calculated by AsteriX-BVI for the imaginery Co(F)(Cl)(Br)(I)(SH)(C=O) organometalic complex. The radius of halogen atoms increases from F to I. The single bond type with cross-section of dodecahedral shape is used for metal complexes. Bond lengths are written in Braille at the panes attached alongside the bonds. The *bottom view* shows the printable label indicating the project and molecules names. The label can be threaded to the 3D model

(e.g., for carbon atoms) or larger (for atoms with larger atomic radii). To decrease finger hindrance, hydrogen atoms can be as small as 0.9 cm in diameter with an associated bond thickness of 0.5 cm. $L_m$, the longest extent in cm of the model and its components $L_x$, $L_y$, $L_z$ in the X, Y, and Z dimensions can be evaluated with two simple formulas:

$$L_m(cm) = L_{ext}(\text{Å})\frac{3.5(cm)}{L_b(\text{Å})} \quad (1)$$

with

$$L_{ext} = \text{Max}[d(i,j)]$$
$$d(i,j) = \textit{distance between any two atoms } i \textit{ and } j$$

and

$$L_b = <L> = \frac{1}{N}\sum_{i=1}^{N}\sum_{j=i+1}^{N-1} l(i,j) \quad (2)$$

with

$$l(i,j) = \textit{bond length between two non} - \textit{hydrogen atoms } i \textit{ and } j$$

$L_x$, $L_y$, $L_z$ are obtained with formula (1) by respectively substituting $|x_i - x_j|$, $|y_i - y_j|$ and $|z_i - z_j|$ for $d(i,j)$ in formula (2).

Because of the relatively small build size of today's printers, the requirement of 3.5 cm for bond lengths does not allow a large molecule as shown in Figs. 8 and 9 to be printed as a whole within the printer build volume, requiring that the model be printed in multiple pieces. The molecule orientation is first rotated to optimally align its long axis relative to the build volume body diagonal. In order to so, the molecule is centred in the build volume and rotated in 1,728 orientations. The orientation for which the molecule goes over the build volume minimally is retained.

If $L_x$, $L_y$ and $L_z$ exceeds the build volume size in the X, Y and Z dimension by <20 %, the molecule is scaled down to fit the printer. If either $L_x$, $L_y$ or $L_z$ exceeds the build volume by more than 20 % the molecule is split in two halves along its longest axis as illustrated in Fig. 8. Bonds that are crossed by the splitting plane are divided in such a way as to provide lock and key complementary shapes that allow unambiguous alignment and gluing of the two halves. This allows models up to 40 cm long to be printed. If the need arises, even larger molecules will be split (the program cannot split them yet in more than two pieces) into more than two pieces, but a quick look at the organic molecules printed over the years in this journal leads us to believe that splitting them once will normally suffice.

## Quantum chemical computation output data representation

To deal with the very large amount of raw data produced by quantum chemical calculations we have integrated in AsteriX-BVI a modified version of the widely used Molden software. Molden is used in nearly ten thousand labs around the world to visualize and analyse the results of quantum chemical calculations, because it can read and process output files from various software suites (e.g., GAUSSIAN, GAMESS, Mopac/Ampac). Result files produced by these quantum chemical programs can be uploaded via the AsteriX web site and processed by Molden in the background. The progression of physical parameters that have been stored in a quantum chemical calculation trajectory (e.g., Maximum Force, Maximum Energy, Maximum Number of Steps per iteration) and that tend to be used to monitor the convergence of a calculation are printed by AsteriX in Braille graphs in the .jpg format and can be directly printed with a regular laser printer on a special thermal paper that, after baking in an oven, produces a relief print (Humanware, developers of PIAF [3]). The figure legend that contains information on the extent of a given curve in the X and the Y direction, the spacing of the X and Y tick marks, and the axis labels are written in Braille on a separate paper sheet. Links to all graphs, figure captions, and haptic models in .stl format are gathered on the project's html page on the AsteriX web site.

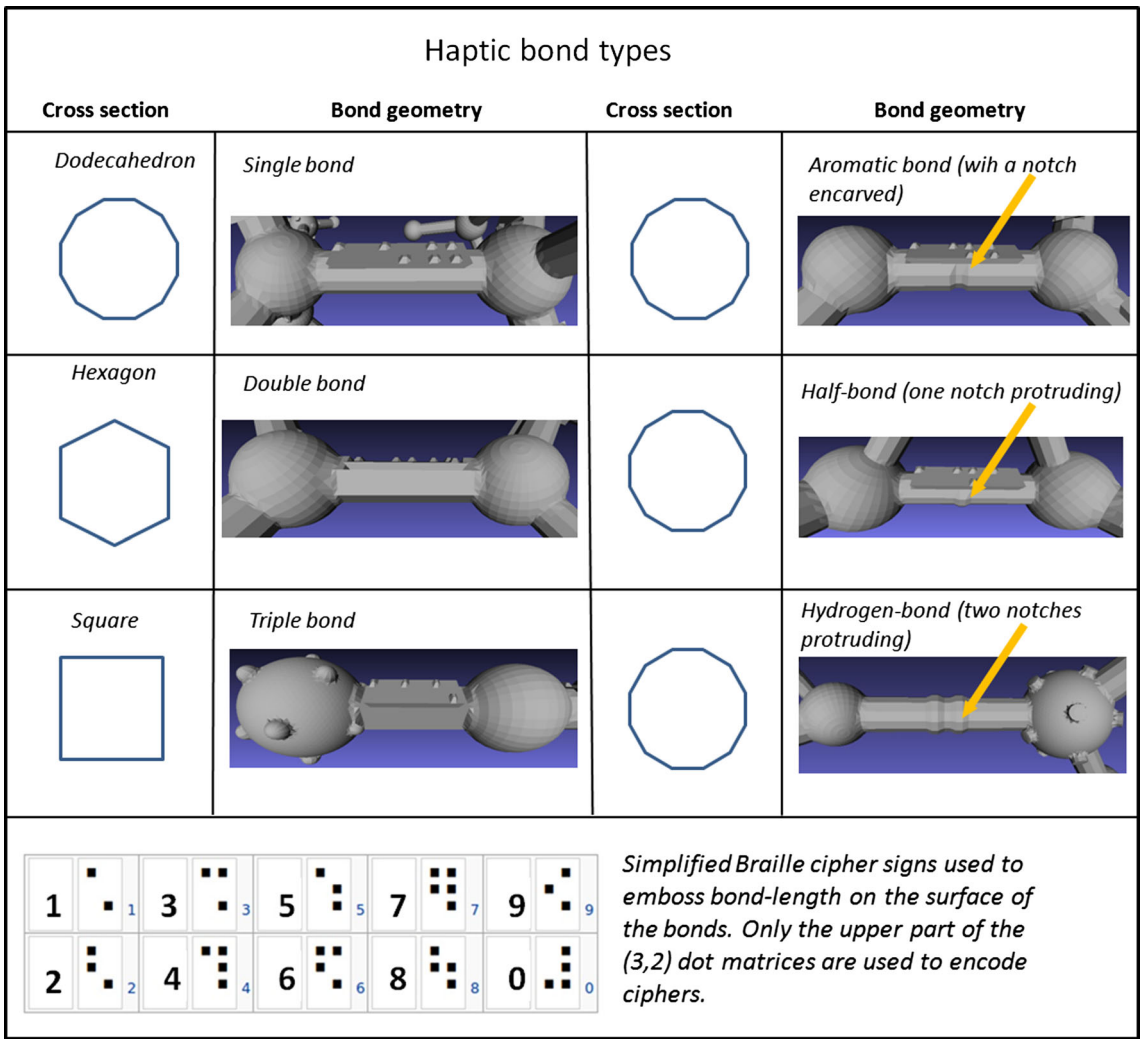


**Fig. 6** Haptic bonds are characterized by particular features that can be easily recognized by the fingers of BVI researchers. Polygonal cross sections as well as the presence or absence of notches in the middle allowed us to define six different bond types. A small pane is generated at the surface of each bond to indicate in Braille its length in 0.01 Å units

The use of AsteriX–BVI is illustrated below with a quantum chemistry project, for which a series of assistive facilities were implemented that manage and allow for visualization of the results of quantum chemical computations. Data files can be uploaded to the server interactively and the Braille (X, Y) curve is produced and annotated in Braille. This methodology may also find application as an accessible graphing calculator for the blind with tactile output via the PIAF.

## Results

The AsteriX–BVI software was applied by HBW to a mechanistic investigation of the heat-induced isomerization of cycloartanol, a carbocationic rearrangement of relevance to the processing of olive oil [14–17]. In tackling this project, the only place where HBW received assistance is with building the initial geometry of a relevant carbocation intermediate using the graphical user interface associated with Gaussian. All computations were performed using the Gaussian 09 software suite [18]. A transition state structure for protonation of a truncated model of cycloartenol was located, as was a subsequent transition state structure for rearrangement of the resulting carbocation. This transition state structure was not described to HBW by an assistant; rather HBW printed it in two parts independently (which he then glued together) and investigated it tactilely (Fig. 9). Upon HBW's assurance that the geometry of the 3D model was satisfactory, along with an accessible investigation of frequency values listed in the Gaussian output file, HBW determined that the 3D-printed structure was indeed a reasonable transition state structure.

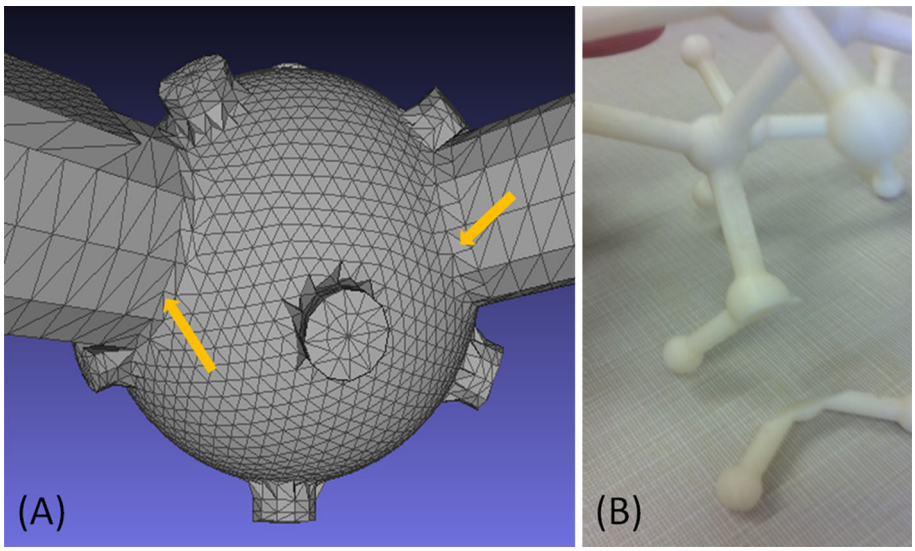


**Fig. 7** **a** Details of the tiling at the intersection between the haptic sphere representing an oxygen atom and the cylinders representing the bonds connected to it. To obtain a closed mesh at the intersection between atoms and bonds, the CAD algorithm adds connecting rings (indicated by *yellow arrows*) at the extremities of every bond cylinder. These rings are covered with a finer mesh that allows a more accurate tiling adjustment. All atom sphere tiles located inside the cylinder cross sections have to be removed. Vertices of the remaining tiles near the connecting rings are adjusted to match the vertices of the closest tiles on the rings. Voids that may appear after this procedure are filled with additional tiles to produce a continuous mesh. The bookkeeping of these voids actually has been the largest programming headache. The algorithm is sufficiently robust to also deal with the connection of the haptic elements to the cylinders and spheres. **b** Example of a printing problem (slicing of the printed model) due to the absence of just a few tiles combined with a couple of misplaced tiles entering inside the surface envelop

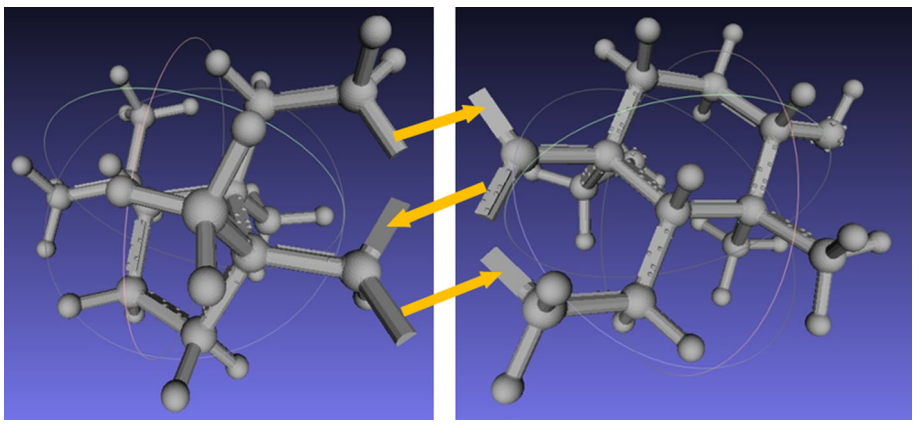

**Fig. 8** Molecules that are too large compared to the build size of the printer are automatically split in two halves along their longest axis. Bonds involved in the splitting process are cut to produce a lock-and-key complementarity (*orange arrows*) that allows them to be reunited unambiguously and glued together easily. The complete 3D model represented by two halves in this splitting image is ~40 cm long (see Fig. 9)

## Discussion

The ability to print highly accurate 3D models of complex objects such as chemical structures that could otherwise only be visualized via a computer screen is opening a new era in assistive technology for BVI scientists. Complex 3D models tailored to fit a particular scientific project in chemistry can now be printed routinely. These models can be prepared automatically via the AsteriX–BVI web site which can be easily accessed and used by BVI users who can enter the molecular structure they study via three different modes: (1) as an image, (2) as a SMILES string, or (3) contained in a GAUSSIAN result file. Integrating several functionalities to provide a comprehensive solution for generating 3D models, analysing the results of quantum chemical calculations, and connecting them to a permanent

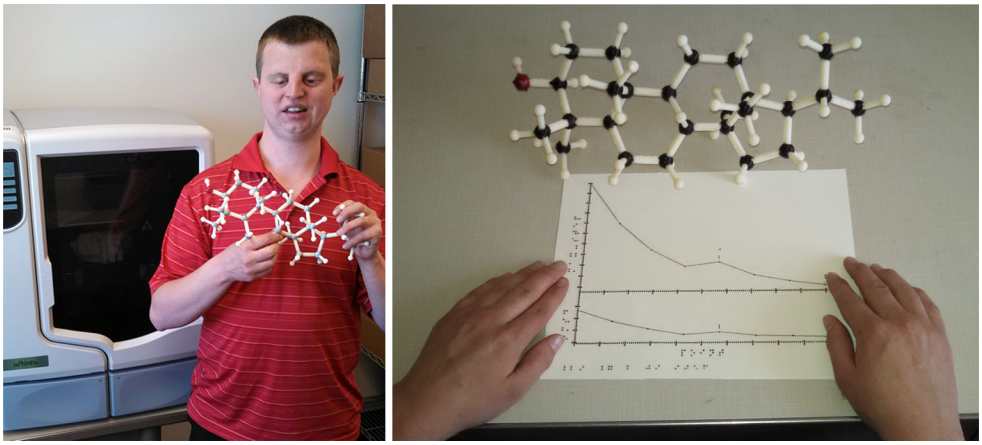

**Fig. 9** *Left* HBW standing in front of a 3D printer holding the 3D model of cycloartenol. *Right* the same 3D model and a Braille graph generated by AsteriX–BVI. They represent the evolution of the maximum number of energy minimization steps along a GAUSSIAN calculation for the cycloartenol transition state structure. The X axis label reads 'POINTS' and the Y axis label 'RMSD' and 'MAX-STEP' for the *lower* and *upper curve*, respectively. Below the X axis label the name of the GAUSSIAN calculation output files is printed. The legend sheet (not shown) includes a summary of the computation output including: the ranges and values of the increments separating the ticks, respectively along the X and Y axes. These Braille graphs can be printed on a special type of paper using a regular office printer. After the sheet of paper is heated in a small oven the relief print of the graph and annotation appears

project space exclusively allocated for the use of a BVI scientist (HBW) was an essential aspect of the success of this project. Inclusion of an efficient molecular editor that can allow BVI users to interactively construct small molecules is the next design task. Work in that direction has been done by another group [19, 20]. Such an editor, however, is yet to be implemented in AsteriX–BVI.

HBW was able to organize, store, and retrieve the scientific information related to his project with efficiency and confidence. The use of a 3D printer paired with the accessible STL generation script has revolutionized HBW's ability to perform computational chemistry at the level of his sighted colleagues. Feeling models and obtaining the same information sighted chemists obtain by looking at a molecular model on a computer screen has proved to be incredibly useful, and it provides a fast method for getting structural information into HBW's mind. In particular, Braille labels indicating bond lengths that correspond directly to a computed molecular geometry provided a useful method for HBW to navigate around a molecule, identify bonds of interest, and to independently perform additional computational chemistry experiments.

The code written to generate .stl files and create 3D models can be expanded to include more haptic markers of atom types that could be designed separately using publically available CAD software and loaded as inputs to our code (in the .stl format). In particular, the creation of special surface textures with different haptic properties could be useful. We would appreciate any collaboration in this direction and we are ready to test and incorporate in our code haptic atom models provided to us in ascii .stl format.

Dealing with ionic bonds and the presence of solvent molecules other than water are areas where we intend to improve our CAD code in the future. Another area of concern is the molecule splitting procedure, which, at this stage, allows only large molecules elongated in one direction (like the sterol shown in Fig. 9) to be printed in two parts with the guarantee that bonds will be glueable. We might in the future need to extend the splitting procedure to generate more than two fragments for large molecules with more complex shapes extending in two or three directions of space.

Colours are a feature that haptic chemical models should incorporate to facilitate efficient communication between BVI and sighted researchers. This is why we have already integrated colours in the .stl files produces by our code.

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