Lab3D online interactive organic chemistry reactions a new molecular visualization resource for undergraduate students

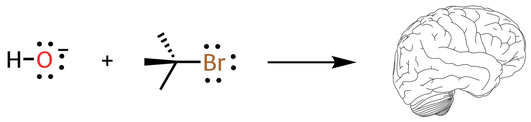
Melanie Burger[1], Michael Corrin[1], Dr Ghislain Deslongchamps[2], Dr Jodie Jenkinson[1]

1. Biomedical Communications, University of Toronto. 2. Department of Chemistry, University of New Brunswick

Master of Science in **Biomedical Communications**

Institute of Medical Science
UNIVERSITY OF TORONTO

Abstract



Lab3D (www.lab3d.me), is a new web-based resource for interactive, animated organic chemistry reactions. **Three-dimensional (3-D) interactive animations** of the sub-micro level **play synchronously alongside 2-D symbolic animations** enabling students to connect the sub-micro and symbolic levels of molecular representation. The objective of Lab3D is to help chemistry learners build dynamic mental models of molecular processes.

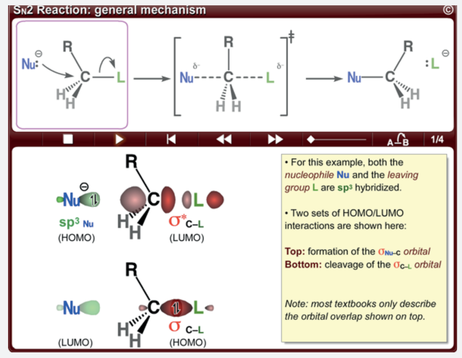
Introduction

Higher student performance in chemistry is linked to visualization skill (Baker, 1972). This reality shapes Lab3D's main goal: to build visualization capacity in chemistry learners. For dynamic processes like molecular reactions, animations are an effective medium (Sanger, 1997). In addition to being animated, **a molecular visualization should be "simple and interactive"**, permitting exploration and manipulation (Williamson, 2005). While the range of molecular processes that can be visualized has been greatly extended by molecular modelling software (Gaussian, Spartan, MOE), molecular modelling plugins within animation software (ePMV, Molecular Maya) and web-based visualization tools (Jmol, ChemDoodle), only the latter permit user interaction and are free for students to use.

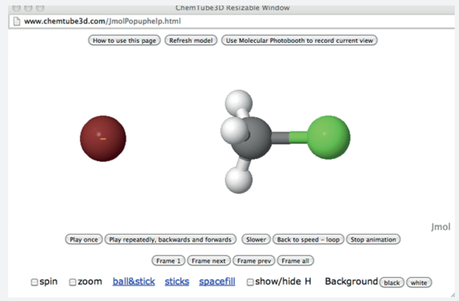
Following guidelines for the effective use of animations in chemistry instruction (Burke, 1998), **animations on Lab3D are short and focussed (< 60s), accurate, allow for student interaction, and are accessible outside of the classroom**. Lab3D is also unique in displaying, side-by-side, synchronized 3-D and 2-D animations. Lab3D is targeted at undergraduate students in their first or second year of organic chemistry and reactions are drawn from the Organic Chemistry 1 curriculum at McGill University.

Inspiration

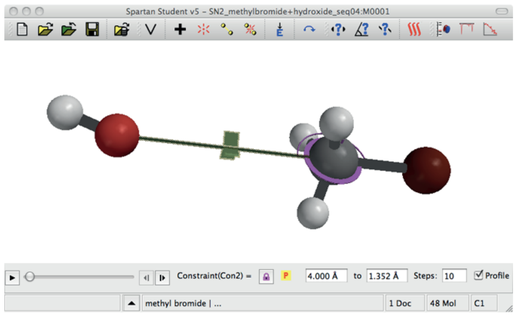
Organic Chemistry Flashware *flashchem.nelson.com*



ChemTube3D *www.chemtube3d.com*

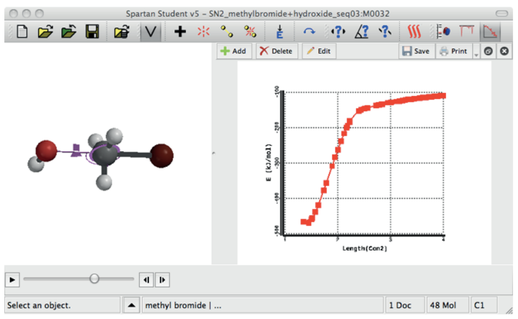


Methods



1 3-D data collection

Reactions were modelled in Spartan Student '10 (Wavefunction Inc.) using a coordinate driven approach at the B3LYP/6-31G* level of theory.



2 3-D data 'work-up'

Energy vs. constraint (internuclear) length was plotted and used to identify the transition state. Bonding information was updated to match and the resulting sequence of structures exported as a MDL SD File. Isodensity surfaces showing electrostatic potential maps were calculated and a movie was generated.

3 Web application

The application framework for Lab3D was developed using HTML5, CSS3, and JavaScript (jQuery v1.9.1). The framework houses the following components:

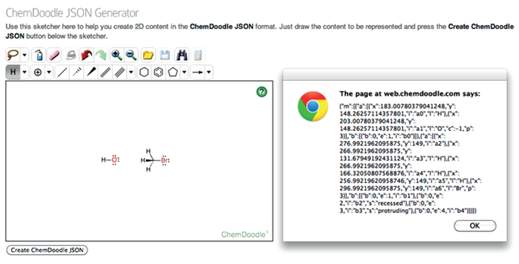
i) 3-D molecular viewer

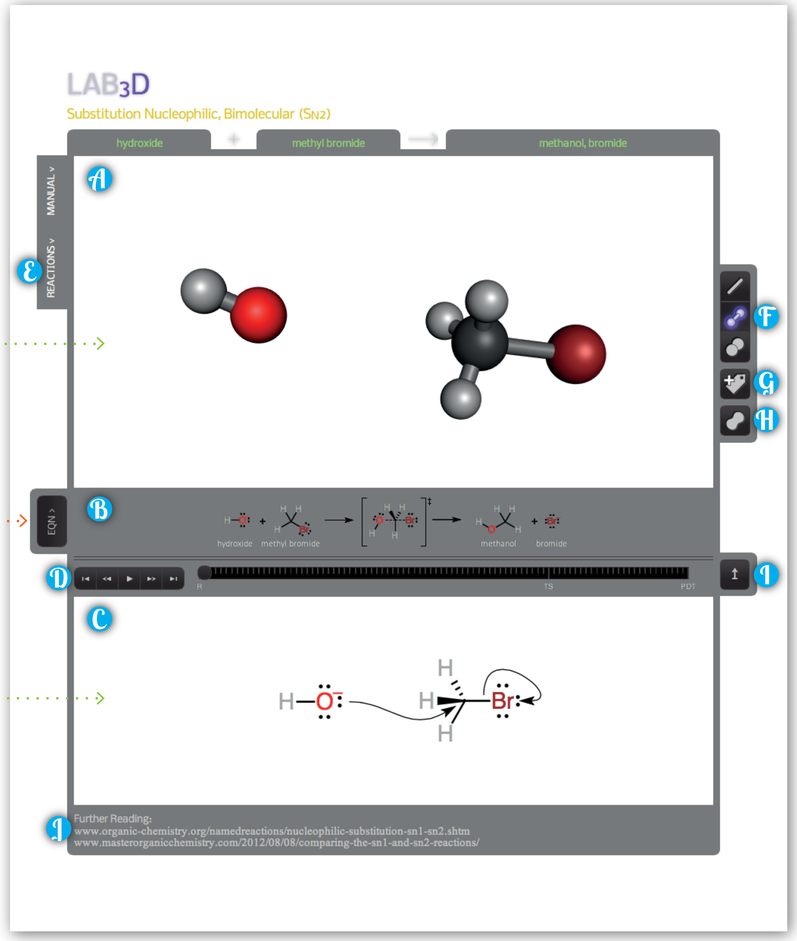
The 3-D viewer uses native Web technologies to load and display molecular graphics data. ChemDoodle Web Components (iChemLabs) was implemented to parse the molecular data (a MDL SD File is retrieved from the server) and generate 3-D WebGL representations.

```
<script>
    //set transition state:
    var TS = 65;
    //initialize canvas:
    var movie = new ChemDoodle.MovieCanvas3D( 'movie', 844, 533 );
    //retrieve MDL SD File:
    ChemDoodle.io.file.content( 'data/SN2_methylbromide%2Bhydroxide.sdf',
    function( fileContent ) {
        //split into MOLFiles (frames):
        var fileArr = fileContent.split( "$$$$\n" );
        var molArr = [];
        for ( var j = 0; j < fileArr.length; j++ ) {
            //parse MOLfiles and generate molecule data structure:
            var mol = ChemDoodle.readMOL( fileArr[j], 1 );
            molArr.push( mol );
        }
        //double the number of frames (optional):
        extMolArr(molArr, TS);
        for ( var i = 0; i < molArr.length; i++ ) {
            movie.addFrame( [molArr[i]], [] );
        }
        //load data into the canvas:
        movie.loadMolecule( movie.frames[0].mols[0] );
    });
</script>
```

ii) Reaction equation

Reaction equations were drawn in the ChemDoodle Web Sketcher and exported for further editing. Additional features were generated using a custom library (Lab3D.js). Finally, the ChemDoodle ViewerCanvas class was used to display the reaction equation in the browser.






```
for ( var i = 0; i < mol1.atoms.length; i++ ){
    //|R*>--------TS--------PDT| (for all slider positions do:)
    //move hydroxide molecule:
    mol1.atoms[i].x = mol1ref.atoms[i].x + ( deltaMove*currSlideVal );
}
if ( currSlideVal > (TS - 10) ) {
    //|R------*>--TS--------PDT|
    //move bromine atom:
    br.x = brRef.x + ( deltaMove*(currSlideVal - (TS - 10)) );
    //create bond between oxygen and carbon:
    if (!this.bondExists(o, c)) {
        mol1.bonds.push(bondOC);
        o.charge = 0;
        o.numLonePair = 2;
    }
}
if ( currSlideVal > (TS - 10) && currSlideVal <= (TS + 10) ) {
    //|R------*>--TS--<*------PDT|
    //move hydrogen atoms:
    h1.x = h1Ref.x + deltaMoveH1*( currSlideVal - (TS - 10) );
    h2.x = h2Ref.x + deltaMoveH2*( currSlideVal - (TS - 10) );
    h3.x = h3Ref.x + deltaMoveH3*( currSlideVal - (TS - 10) );
}
if ( currSlideVal > (TS + 10) ) {
    //|R--------TS--*>-------PDT|
    //remove bond between carbon and bromine:
    if (this.bondExists(c, br)) {
        bondCBr = mol2.bonds.splice(0,1)[0];
        br.charge = -1;
        br.numLonePair = 4;
    }
}
```

iii) 2-D symbolic animations and viewer

The 2-D animation sequence was storyboarded. Initial HTML5-ready JavaScript objects (symbolic representation) were generated using the ChemDoodle Web Sketcher. The 2-D animation was scripted from these initial coordinates. Atom movement, bond breaking, forming and order changes, and curly arrows were programmed to closely follow the 3-D animation. A custom extension of ChemDoodle's AnimatorCanvas class was used to play animations.

Walkthrough

A 3-D animation viewer. As the animation plays, the scene can be rotated, translated, and scaled.

B The overall reaction equation is shown by default, but can also be hidden from view.

C 2-D animation viewer.

D The animations are controlled through the media controls and slider. Play, pause, advance or rewind by a frame, move to the start or end, and scrub through the animation at your own speed. The slider functions as a reaction coordinate, showing the location of transition states.

E From a list of general reaction categories, select a set of reactants

F Toggle stick, ball-and-stick, and CPK representations.

G Toggle atom labels.

H Click to play a movie of the reaction with a surface representation.

I Click and drag to adjust the height of the 3-D viewer and bring the 2-D viewer "above the fold" of the browser window.

J Curated, contextual links are provided for additional information about each reaction.

A Novel Representation?

Present day 3-D graphics applications open new possibilities for molecular visualization. For example, a new 3-D representation could show electrons explicitly and help students to rationalize mechanisms. Showing frontier orbitals could clarify reaction stereochemistry but might also create too complex visual displays. It is not yet clear what a novel representation might look like, only that there is room for one that may offer additional pedagogical value and reduce misconceptions in chemistry (Tasker, 2008).

Future Directions

Short-term

- Expand Lab3D's collection of visualized reactions.

Long Term

- Develop a surface representation for WebGL scenes that can map electrostatic potential and other properties.
- Build a ChemDoodle 2-D Animation Sketcher. The sketcher would be capable of importing 3-D molecular data to initialize key frames for 2-D animations. The user would be able to customize and key atom position, lone pairs, curly arrows, etc.
- Seek partners in chemistry education to incorporate Lab3D into their curriculum and facilitate its study. Areas of research interest include impact on visuospatial reasoning, and changes in common misconceptions and achievement in chemistry.

References

Baker, S. R., Talley, L. (1972). The relationship of visualization skills to achievements in freshman chemistry. *J. Chem. Ed.*, 49(11), 775.

Sanger, M. J., & Greenbowe, T. J. (1997). Students' misconceptions in electrochemistry regarding current flow in electrolyte solutions and the salt bridge. *J. Chem. Ed.*, 74(7), 819.

Williamson, T. (2005). Molecular Visualization in Science Education: An Evaluation of the NSF-Sponsored Workshop, *J. Chem. Ed.*, 82(6),1–7.

Burke, K. A., Greenbowe, T. J., Windschitl, M.A. (1998). Developing and using conceptual computer animations for chemistry instruction. *J. Chem. Ed.*, 75(12), 1658–1661.

Tasker, R., Dalton, R. (2008). Visualizing the molecular world – design, evaluation, and use of animations. *Visualization: Theory and practice in science education*, 103–131.

Support

CIHR IRSC Canadian Institutes of Health Research / Instituts de recherche en santé du Canada

Ontario