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Dynamic Representation of Organic Chemical Reaction Mechanisms with Animated Lewis Structures

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Abstract Animations and Simulations are suitable to explain chemical facts. In 2011 the new 2D structure editor MyChemise was introduced by the author. After upgrading to a new version the software is now offering the possibility to export animations as gif files. Through the use of 2D animations, it is possible to visualize depictions of reaction mechanisms for digital media. With the free available software MyChemise they can be developed in a simple manner within a relatively short amount of time. The exported gif files offer many ways to make use of the animations. In Wikipedia articles, these animations illustrate the chemical processes described in the text and complement conventional sketches. The new kusGifViewer allows to control the representation for educational purposes.

Keywords: *2D animations, reaction mechanisms, digital media, MyChemise, kusGifViewer*

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1. Introduction

Chemical processes can be illustrated by computer animations, and these animations are widespread in many fields of chemistry [1,2,3]. There is a large varied range of animations offered online covering different areas of chemistry, e.g., for school education and introductory lectures (see, e.g., [4,5,6]). In addition, the publishers of science textbooks offer animations to supplement the printed material (see, e.g., [7]).

2D and 3D animations are suitable for the presentation of reaction mechanisms on a PC. With appropriate tools, 3D technology can be used on the web to demonstrate changes in chemical structures on a molecular level in a spatial manner [8,9,10,11,12,13]. 2D animations are especially suitable for schematic depictions of mechanisms on a symbolic level [14]. A disadvantage of most of these animations is the requirement of a special program or plug in to show the animations. Furthermore, there is only a limited selection of animations available, and it is often not free to download them.

Therefore it appeared worthwhile to provide a tool which allows to generate such animations by everyone. That is why the existing software got an appropriate extension. Over 60 animations of chemical reaction mechanisms were created during the last three years and the result of this work is presented in the following.

2. Creating Animations

The former described [15] and self-programmed software MyChemise exists meanwhile in the sixth version. It is a free online Java program that can produce 2D animations of reaction mechanisms with animated Lewis structures. The atom displacements that occur during the reaction are shown with this tool. The chemical content can be flexibly demonstrated through the use of different colors for various types of atoms and by fading in or out matching background images. For creating an animation, only single reaction steps have to be drawn.

The most important part during the development process of an animation is the exact marking of the correlating areas in the two reaction stages (Figure 1). These areas are morphed by the software.

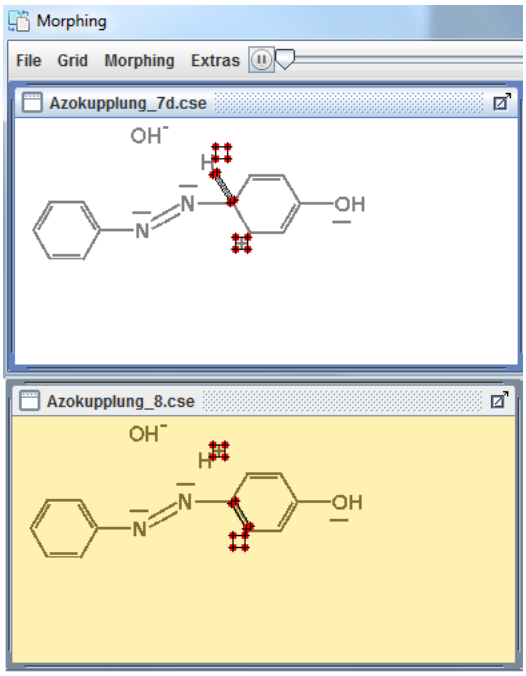

Figure 1. The morphing window of MyChemise with marked areas

The speed of the animation can be controlled by the number and duration of the numerous intermediate images that make the transitions smoother.

These images are calculated by the MyChemise program, which is why animations can be generated quickly. The morphing process itself is realized using the unit squares method [16]. A software description [17] with an introduction how to make animations and many examples of animated chemical reaction mechanisms can be found on the author's homepage [18].

3. Using Animations

3.1. In Articles

The animations can be exported as animated gif files which is possible since the release of the second version of MyChemise. In this way they can be used directly in many digital ways, e.g., screen presentations (or in the HTML version of this text, Figure 2) without any further tools.

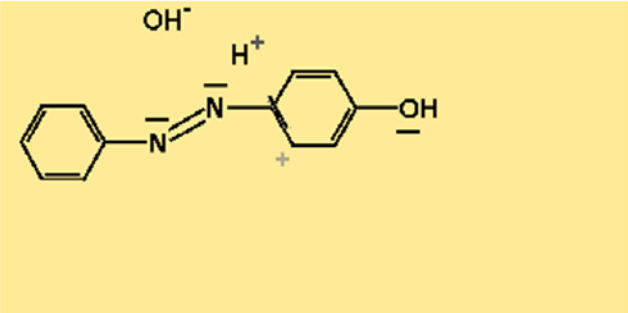

Figure 2. Gif animation of the Azo coupling

More than 30 (October 2015) animations are embedded in Wikipedia articles of named chemical reactions in various languages. The animations are pictured as endless loops and consist of up to 1500 single frames. Each cycle lasts between 0.5 and 2 minutes. All animations are saved at Wikimedia Commons [19] and are used in the articles in different ways. The direct embedding of the animations into the text [20] enables the reader to look at the sketches and the animations at a glance. It is advantageous when the gif files can be interrupted by installing an add-on which is available for some browsers (Figure 3).

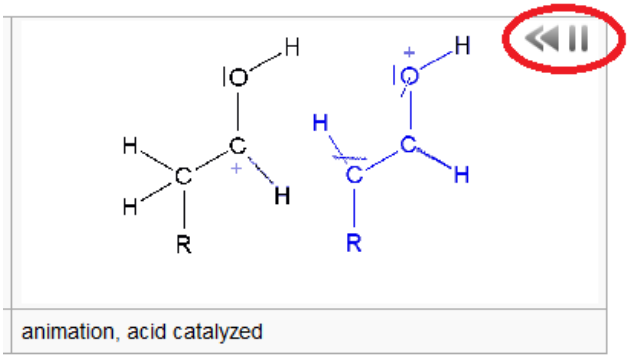

Figure 3. Screenshot of the Wikipedia Aldol condensation article [21] on a browser with installed add-on showing the animation with control elements (marked red)

Separation of the graphics from the text can be realized by placing a frame around the animations [22] or by adding them into a new section. It is a better way to insert them as external links [23] if the animations vary slightly (e.g., different side chains) from the sketches or differ from the optical appearance of the text (see Mesaros [24] for a description about the interaction of animations in German Wikipedia articles).

3.2. The kusGifViewer

A new interactive gif viewer (Figure 4) was created by the author in order to provide the animations for educational purposes (presentations, lectures) in offline mode, too.

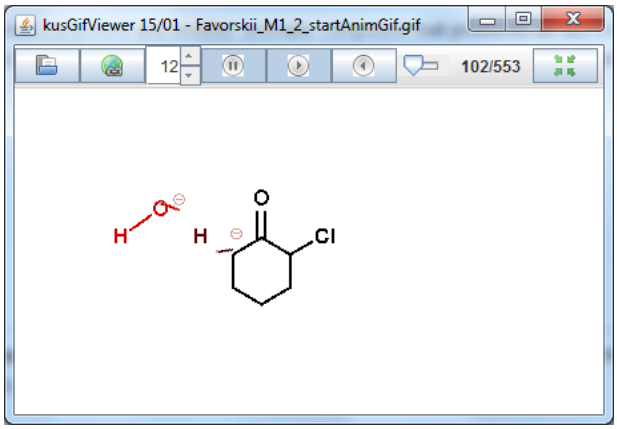

Figure 4. The kusGifViewer with a screenshot of the Favorskii rearrangement

This Java application makes it possible to start and stop the visualization. Furthermore the running direction and the pacing can be adapted to personal needs. With a click on its surface one can select an undecorated style, without the menu bar and without frame. The author's homepage [18] offers the kusGifViewer for free download.

3.3. Advantages of the Animations

Text, depictions and animations complement each other ideally when they are closely coordinated. For advanced learners, the animations can open up new perspectives on the reactions.

These animations were developed to show the reaction mechanisms in clear manner and they are a bridge between static printed sketches and the 3D animations. Even extensive reaction mechanisms can be placed in the text without dissecting it too much because they are only the size of a Lewis structure.

MyChemise enables everybody to construct animations on their own although it is not easy at the beginning. When developing a new animation for the first time, it is necessary to learn how to use the software apart from needing knowledge of the reaction itself. However, it is a challenge to obtain a good animation as a result of careful work.

4. Conclusions

The visualization of reaction mechanisms with animated Lewis structures is a good option to complement the well-known depictions from printed media when using the animations in audiovisual media. Even more complex

reactions can be shown in this manner and due to the free availability of the described software, they can be widely used. Studies with students showed that using interactive animations had a positive effect on their understanding [25,26]. Therefore, it may be helpful for learning to present the reaction mechanisms in this way. For this purpose a learning software is currently being developed and will be available in the next months.

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To my sister and to my brother.
And thanks again to my family.

References

[1] Suits, J. P., Sanger, M. J., Eds, *Pedagogic Roles of Animations and Simulations in Chemistry Courses*, *ACS Symposium Series 1142*, American Chemical Society, Washington, DC, 2013.

[2] Tasker, R, Dalton, R., "Research into practice: visualisation of the molecular world using animations," *Chem. Educ. Res. Pract*., 7(2), 141-159, 2006.

[3] Welsch, N., Meyer, C., Albert, K., "Bilder sagen mehr als tausend Worte: Visualisierungen für Lehre und Forschung," C*hem. Unserer Zeit*, 40, 316-325, 2006.

[4] University of Colorado, PhET. Available: *https://phet.colorado.edu/en/simulations/category/chemistry* (accessed December 2015).

[5] Bergische-Universität Wuppertal, Chemie interaktiv. Available: *http://www.chemie-interaktiv.net/ff.htm* (accessed December 2015).

[6] Australian University Teaching Committee (AUTC), VisChem Animations.Available: *http://learningdesigns.uow.edu.au/tools/info/T4/index.html* (accessed December 2015).

[7] Wiley, Fundamentals of Biochemistry. Available: http://www.wiley.com/college/fob/anim/index.html (accessed December 2015).

[8] Muzyka, J. L., "Visualization Tools for Organic Chemistry," *J. Chem. Educ*., 40, 86 (2), 254, 2009.

[9] Höfker, U., "3D-Reaktionsanimationen im Netz," C*hem. Unserer Zeit*, 37, 220-221, 2003.

[10] Borkent, H., van Rooij, J., Stueker, O., Brunberg, I., Fels, G., "Web-Based Computations and Animations," *J. Chem. Educ*., 80 (5), 583, 2003.

[11] Wiley Information Services GmbH, ChemgaPedia. Available: *http://www.chemgapedia.de/vsengine/vlu/vsc/de/ch/2/vlu/anim/3d_anim.vlu.html* (accessed December 2015).

[12] University of Liverpool, ChemTube3D. Available: *http://www.chemtube3d.com* (accessed December 2015).

[13] Radboud Universiteit Nijmegen, Mol4D. Available: *http://wetche.cmbi.ru.nl/organic/index.html* (accessed December 2015).

[14] University of Hildesheim, ChiLe. Available: http://www.chemieunterricht-interaktiv.de/en/pages/animations/animations_2d.html (accessed December 2015).

[15] Wilhelm, J.-H, MyChemise: "A 2D drawing program that uses morphing for visualisation purposes," *J. Cheminform*.., 3:53, 2011. Available: *http://www.jcheminf.com/content/3/1/53*l (accessed December 2015).

[16] Burger, W., Burge, M.J., *Digitale Bildverarbeitung*, Springer-Verlag, Berlin, 2005, 377-385.

[17] Wilhelm, J.-H., MyChemise description. Available: http://www.knalltundstinkt.de/MyChemise_englisch/Description.pdf (accessed December 2015).

[18] Wilhelm, J.-H., homepage. Available: http://knalltundstinkt.de/englische%20Version/knalltundstinktE.html (accessed December 2015).

[19] Wikimedia Commons user contributions of the author. Available: https://commons.wikimedia.org/wiki/Special:Contributions/Kus2014 (accessed December 2015).

[20] Wikipedia, Esterification. Available: https://ru.wikipedia.org/wiki/%D0%AD%D1%82%D0%B5%D1%80%D0%B8%D1%84%D0%B8%D0%BA%D0%B0%D1%86%D0%B8%D1%8F (accessed December 2015).

[21] Wikipedia Aldol condensation. Available: https://en.wikipedia.org/wiki/Aldol_condensation (accessed December 2015).

[22] Wikipedia, Hydroboration. Available: https://pl.wikipedia.org/wiki/Hydroborowanie (accessed December 2015).

[23] Wikipedia, Hofmann elimination. Available: https://es.wikipedia.org/wiki/Eliminaci%C3%B3n_de_Hofmann (accessed December 2015).

[24] Mesaros, M., *Ersterstellung und Optimierung chemiebezogener Artikel in der Wikipedia-Enzyklopädie*, Bachelor thesis, Carl von Ossietzky Universität, Oldenburg, Germany, 2014.

[25] Akaygun, S., Jones, L., "Animation or Simulation: Investigating the Importance of Interactivity for Learnimng Solubility Equilibria," in [1], 127-159.

[26] Weitz, D. A., "Effectiveness of Animation as a Learning Strategy in a Classical Control Theory Introductory Course," *World Journal Control Science and Engineering* 3.1, 8-12, 2015. Available: http://pubs.sciepub.com/wjcse/3/1/2/index.html (accessed December 2015).