Rhorix - Quick Start Guide

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Rhorix is an add-on (plugin) program that allows users to draw (in 3D space) and render (in 2D flatland) a representation of the quantum chemical topology (QCT) of a chemical system with the powerful Blender[1] tool. This 'Quick Start' document is intended for those users currently without interest in how the program works who simply want to get started making images. The quickest path from QCT calculation to rendered picture is discussed, explaining how to immediately start using Rhorix with Blender to generate a standard-appearance rendered image from a QCT data file.

Those users requiring more detail should consult the Rhorix paper[2] and Blender Manual[3]. All users are urged to first look therein for answers not present in this guide before contacting the author[4].

[1] www.blender.org

[2] Mills, Sale, Simmons, Popelier, J. Comput. Chem., 2017, 38(29), 2538-2552

[3] www.blender.org/manual/

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Obtaining the Program

The source code for Rhorix can be downloaded from the release page on GitHub[5]. The supplied archive contains the Blender Add-On Python code, an XML document type definition file, filetype conversion Perl scripts, example projects and documentation.

[5] github.com/MJLMills/rhorix

Installing the Add-On

The currently supported version (2.79) of Blender must be installed before proceeding with the Rhorix installation. Installing Blender is not covered here; please consult their website[6] for instructions for your OS[7]. Once a working version of Blender is in place, the script can be installed within it.

[6] www.blender.org/download

[7] Windows, Mac OSX, GNU/Linux and FreeBSD are supported.

Installation of the script requires the program contents be extracted into their own directory within the Blender addons directory, the location of which is OS-dependent. After placing the files in the appropriate location, open Blender, navigate to User Preferences in the File menu and choose the Add-Ons tab[8]. Use the search box to find Rhorix. To activate, tick the checkbox to the left of the entry. The Blender configuration can be saved for all future documents[9], or alternatively the Add-On can be re-ticked in each new document used for QCT drawing. The script, when the checkbox is selected, will add the ability to read an XML topology file into Blender in various places.

[8] File → User Preferences → Add-Ons

[9] Ctrl+U

Converting QCT Output Files

In order to model and render a topology, the topology must first be known. Therefore, a charge density analysis calculation is the first step in producing an image. Instructions on producing the data necessary to render an image of the topology should be found in the documentation of your particular QCT analysis program. Rhorix currently supports MORPHY (mif) and AIMAll (viz) output files (and by extension supports any *ab initio* code that produces an AIM wavefunction), which must be converted to the .top filetype before they can be read into Blender. Several Perl scripts are provided for this purpose, named for the filetype that they convert from. The Readme file in the appropriate program directory gives detailed information on using these scripts.

Reading Topology Files

After successful conversion, the .top file can be read into Blender via Rhorix by clicking the appropriate menu item[10] and navigating to the file's location. The appearance of the topology will follow the default mapping described in the paper, i.e. standard colors and sphere radii will be used. Following successful reading of a .top file, a 3D model of the topology will appear in the View window.

[10] File → Import → Quantum Chemical Topology (.top)

Useful GUI Buttons

Rhorix provides a set of useful buttons for commonly needed manipulation tasks. These can be used to select and resize various types of gradient path, turn on or off all CPs of a given type and switch to stereoscopic rendering. The buttons can be found in the left-hand pane under Tools.

Placing the Camera & Rendering an Image

The camera must be positioned such that the appropriate part of the topology will be rendered onto the 2D image plane. Rendering can be imagined as the process of taking a picture of the topology with the virtual camera, and so all of the camera settings affect the outcome. Rhorix automatically positions the camera such that it is outside the system and points at the origin. This is intended to provide an adequate starting point only. A simple three-point lighting system is also created.

The user is referred to the appropriate sections of the Blender documentation for descriptions of the camera settings. The mini-

mal demand on the user is typically to move the camera to get the desired part of the system in the final render.

There are 2 important 3D viewports for the quickstart user. The program will show the 3D view window once the system is read in. The purpose of this view is to allow the manipulation of objects and materials, and provide a pre-rendered image of the scene. The second viewport is the Camera View. The camera view shows you the orientation of the objects which will be rendered to the final image. Thus you should check that your system appears correctly drawn in the 3D view first, and then enter the camera view mode to set the viewpoint of your final 3D render.

To move the camera, it is recommended that you enter the camera view mode[11], and then use the fly mode[12] to position the camera using your mouse. The enter key freezes the camera when you find the viewpoint that you want. For larger systems, the z-clipping (which hides objects from the view deemed too far from the camera) will eliminate parts of your system. If this happens, select the camera, and then its object data panel. Increase the value of 'End' in the 'Clipping' section until the part of your scene you want returns to the camera view. Pressing the F12 key will invoke the Blender Render engine and produce a rendered image of your scene from the chosen viewpoint. The Esc key leaves the render mode if you want to make further changes.

[11] keypad 0

[12] Shift-F

The camera can be moved in other ways once in camera view mode. Please see link[13] for more details.

[13] www.blender.org/manual/editors/3dview/navigate/ca

Manipulating Appearance

Summary

The above information constitutes the minimum required to produce a Rhorix image from a QCT calculation output file. For further information on the theoretical background and function of RhoRix, please consult the Manual. For a detailed description of the implementation please consult the paper describing this work[14].

It is hoped that the program website[15] will become a repository of completed images and example .blend files in order to inform and inspire future work. Please consider sharing your final Blender save file and rendered image with us, as well as the location of any publications that use this software. If you use Rhorix, please give credit by citing both the Rhorix paper and the program (as Rhorix - A Program for Drawing of Quantum Chemical Topologies by M J L Mills, www.mjohnmills.com/rhorix) where appropriate.

[14] Mills, Sale, Simmons, Popelier, J. Comput. Chem., 2017, 38(29), 2538-2552

[15] www.mjohnmills.com/rhorix