**Chemical Structure Simulator (CSS)** Documentation

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# Introduction

## Purpose of the documentation

The purpose of this document is to allow the user to fully understand all the features of the application and how to effectively make use of them.

## How to use this document

The documentation is split into different sections. Each section will contain a single feature. Each section will be further divided into multiple subsections: general summary of the feature, how to use it, what to expect from it, and a more technical description of the feature. At the end of this document, there will be a list of shortcuts that can be used in the application to speed up some tasks. In the appendix, there will be the features of the algorithms.

# Prerequisites

## Getting this application

The entirety of this application, along with the optional source code, is available on GitHub. To install the executable and/or the source code, please visit and clone:

<https://github.com/volovikariel/ChemicalSimulator>

## Dependencies

### Java

To run this application natively on Java (using the jar file instead of the executable), the computer running this application must also have JRE (Java Runtime Environment) installed. Otherwise, the user must use the executable (\*.exe, \*.out).

## Specifications

Since the algorithm this application is based on is a very broad and thus very computationally expensive, it is highly recommended to have at least 2GB of memory available on the device.

# Features

The features that follow are all features that affect the user directly, sparing the overly technical descriptions of the algorithms, which are accessible in the appendix.

## Periodic Table

### Summary

The Periodic Table is available as a form of reference, and as a form of input for the user.

### How to use

The user can drag and drop individual atoms into the top portion of the screen, this will add it to the list of atoms that will be considered for the algorithm. The user can also right click to remove them, or alternatively drag and drop them back into the periodic table. The user can also delete individual atoms by pressing backspace after having added it.

### What to expect

The user can expect intuitive controls for the addition and removal of atoms. The user can also expect to have a periodic table which looks familiar to the one they’re used to, that is to say: it is ordered in the standard form so that the user knows what column the atom is situated in, it is colour coded to facilitate finding metals and non-metals and other subgroups, it shows the atom’s atomic number. [POSSIBLY ADD MORE INFO LIKE ATOMIC MASS WHEN IT MATTERS IN ALGORITHM]

### Technical Description

## Text Input

### Summary

### How to use

### What to expect

### Technical Description

## Loading Screen

### Summary

### How to use

### What to expect

### Technical Description

## Tabs

### Summary

### How to use

### What to expect

### Technical Description

## Lewis Structure

### Summary

### How to use

### What to expect

### Technical Description

## Three-Dimensional Display

### Summary

The Three-Dimensional Display is a 3D representation of the chemical compound (the *group*).

### How to use

The *group* can be **rotated** by pressing down the primary mouse button and moving the cursor.

The *group* can be **translated**/**moved** by pressing down the secondary mouse button (usually the right) and moving the cursor to where you want the group to be.

*group* can be **zoomed in and out** by using the scroll wheel.

A *group’s* atom can be hovered over and its **symbol** will be **displayed** at the bottom of the screen.

### What to expect

The user can expect the angles between atoms to be close to what they are theoretically.

The user can expect to see the proper bond counts for each solution.

The user can expect to see the formal charge on each atom if it is not neutral.

The atoms are distinguishable one from the other, for instance hydrogen atoms as seen in the group are of a lighter colour and of a smaller size. The user can also display its symbol by hovering over it.

### Technical Description

# Shortcuts

# Appendix

## Structures

## Sorting