

Additional Reading Material

Tutorial Title: Superimposing Structures

(I) The Cahn-Ingold-Prelog rules

<https://myheplus.com/uploads/stcS3lSCgPZOMApNs6MilzaRTtADBD7KUHzno6Lm.pdf>

These rules give the absolute configuration, R and S for each chiral center within a compound. The chiral centers are named either R or S.

To name a chiral center using the Cahn-Ingold-Prelog rules:

- 1) Identify a carbon with four different groups attached to it.
- 2) Put the lightest group at the back (i.e. pointing away from you).
- 3) Give the heaviest group attached to the chiral center highest priority, number 1.
- 4) Give the second heaviest group attached the number 2.
- 5) Give the third heaviest group attached the number 3.
- 6) If, with the lightest group or atom pointing away from you, the highest priority to the lowest priority (1 to 2 to 3) goes clockwise, the center is named R, counterclockwise it is called S.
- 7) When looking for the heaviest group/atom you start with the atom joined to the chiral center if they are all different, just put them in order of atomic mass.
- 8) If you have two same groups, look for the atom which differs in the group and prioritize the groups accordingly.

(II) Steps to change the default directory to save files in Jmol.

1. Open the **Console** in Jmol (**Console** is available as an option in the **File** menu).
2. Any of the following Commands can be used to set the path to load or save files. In the Double-quotes, in place of "**path**" or "**directory path**" type your preferred path.

(i) **set currentLocalPath "path"**

(ii) **set defaultDirectory "directory path"**

Examples: If I need to save or upload files from **Downloads** folder under user name **Spoken** in **Users** directory, in the Console window at the prompt type,

```
set defaultDirectory "/Users/spoken/Downloads"
```

For example if your user home directory is "**Ada**", in the **Console** window at the prompt type,

```
set defaultDirectory "/home/Ada/"
```

For more information on Set command (Set (Files and Scripts) use the link given below.

<https://chemapps.stolaf.edu/jmol/docs/#set>

