## horizontal line



Crystal splicer

28.06.2018

**─**

AJH

Mancheter One

Portland Street

# Overview

Hello! This is a crystal splicer script, its works by taking a particular conformer and adding it into the structure. Each folder should contain the necessary information to run each script, however, here are some key points you need to know before running this script:

# Things to note before running script:

* Make a backup of the project

# Things that you need:

* Gyrate file, currentIC file, crystal structure which has been correctly labelled

# Mechanism: What the script does

* Takes gyrate file; builds DoF tree,
* Take currentIC file: finds torsions,
* Takes SDF file; measure key angles,
* Makes changes to gyrate file