generalInstructions

# Description

How to perform quantum calculations

# Part 1: General Instructions

## Submit Job

**Instructions on how to build a molecule, submit a job, and view the results.**

Make sure you are logged in. Registered users are allocated more computational power.

Click the next button to begin!

**There are three ways to build a molecule:**

Type the name of the molecule in the box the left and press Enter.

Right click on the window to the left and paste a mol or Smiles description.

Draw the molecule using the interface to the left.

Use the +/- icon to set the charge on an atom.

Use the X element for hydrogen or other atoms not listed.

Note: You can also hover your mouse and hit the h-key for hydrogen

**Once the molecule is drawn in 2D you convert it to 3D for submission:**

Click the Transfer Button to convert the molecule to 3D

It will automatically be optimized and symmetrized

**Set Calculation Parameters:**

Click Reset Settings to Default to start

Enter a name for your input file, e.g. H2\_lastname

Set your job options. Help is provided at the left for some options.

Click "Submit Job"

Measurements can be made by double clicking on an atom to start and stop a measurement. Single click on intermediate atoms to measure angles

## Analyze Results

**Visualize Your Results**

Write down your job number (6 digit number at the left). Wait for the job to finish.

Under visualizations choose to view orbitals or vibrations (if calculated in the previous step)

Measurements can be made by double clicking on an atom to start and stop a measurement. Single click on intermediate atoms to measure angles

To perform additional calculations using this molecule click "Do More Calculations"

To perform calculations on a new molecule click the Submit Tab at the top.