

## MCTDH Summer School, Heidelberg July 2025

### Preparing for the Tutorials

In addition to a standard linux environment with a python3 interpreter, you will need

- A Fortran compiler. Best is a recent version of gfortran.
- The fortran sqlite libraries. These are in the linux packages sqlite3 and sqlite3-devel.
- gnuplot (version 5 is better, but version 4 can be used).
- jmol

It is assumed that you use a bash shell, and adjustments will have to be made if a different shell is used.

#### 1. Install Quantics.

- Download `quantics_package.tar.gz` from `www.chem.ucl.ac.uk/quantics` under **Tutorial Package** into your home directory

- extract using

```
gunzip quantics_package.tar.gz
tar xvf quantics_package.tar
```

- This will have created a directory **quantics\_package**
- install

```
cd quantics_package/install
.\install_quantics -y
```

This will take a few minutes and hopefully everything will compile without problems. You will need to set up the environment variables by (assuming you are using a bash shell) typing

```
source ~/.bashrc
```

In future the activation will be automatic on login.

#### 2. Install Gaussian09

- Download `g09exe.tar.gz` from `www.chem.ucl.ac.uk/quantics` under **Tutorial QC Package** into your home directory

- extract using

```
gunzip g09exe.tar.gz
tar xvf g09exe.tar
```

- This will have created a directory **g09exe**

- copy the file run\_g09 (in the Tutorial Supporting Files) to your bin directory. Edit the paths in run\_g09 to fit your installation. All that should be required is to replace XXX in the following lines with your home directory

```
g09root="/home/XXX/g09exe"  
GAUSS_SCRDIR="/home/XXX/scratch"
```

The directory GAUSS\_SCRDIR needs to be created with mkdir.

### 3. Install JMol

- Download jmol.tar.gz from [www.chem.ucl.ac.uk/quantics](http://www.chem.ucl.ac.uk/quantics) under **Tutorial JMol Package** into your bin directory
- extract using

```
gunzip jmol.tar.gz  
tar xvf jmol.tar
```

- edit the following line in the file bin/jmol to add the correct home directory

```
export JMOL_HOME="/home/XXX/bin/jmol-13.0.16"
```