For the tutorial "Rotational Spectroscopy for Radioastronomy" by S. Brünken you need to install the software PGOPHER on your own laptop prior to the course. The following gives a brief guide on how to install it.

Quick guide to install PGOPHER

PGOPHER is a free open source program written and maintained by Colin Western (University of Bristol) for simulating and fitting rotational, vibrational, and electronic molecular spectra (Western 2017). There is a website where the program can be downloaded and where additional information and support (online manual) can be found: <u>http://pgopher.chm.bris.ac.uk/</u>

The program is very powerful and can be used to

- a) Analyse an experimental spectrum by fitting spectroscopic constants to the data
- b) Use known spectroscopic constants to simulate a spectrum

It can be used for electronic, vibrational, and rotational data. In the tutorial we will work only with rotational data. We will learn how to analyse a simple experimental spectrum and then how to predict the rotational transition frequencies of a molecule that you, e.g., want to search for in space.

- 1. Download Pgopher from the website http://pgopher.chm.bris.ac.uk/
 - Go to Download, read the readme.htm or readme.txt
 - Windows: safe PgopherU64.exe (for 64bit machines) or Pgopher.exe (for 32bit machines) together with pgopher.chm in any convenient folder, see http://pgopher.chm.bris.ac.uk/Help/installwin.htm for further instructions.
 - Mac: download and unzip pgopher-MacOSX-i386-carbon.app.zip and install (needs OS X Leopard (10.5) or above), see http://pgopher.chm.bris.ac.uk/Help/installmac.htm for further instructions. If you use OS X Catalina (10.15) you need to install the development Version pgopher-MacOSX-x86_64-cocoa.app.zip that can be found here: http://pgopher.chm.bris.ac.uk/pgopher.chm.bris.ac.uk/pgopher.chm.bris.ac.uk/pgopher.chm.bris.ac.uk/pgopher.chm.bris.ac.uk/pgopher.chm.bris.ac.uk/pgopher.chm.bris.ac.uk/pgopher.chm.bris.ac.uk/pgopher.chm.bris.ac.uk/pgopher.chm.bris.ac.uk/pgopher.chm.bris.ac.uk/pgopher.beta/pgopher.MacOSX-x86_64-cocoa.app.zip
 - Linux: download and unzip pgopher-x86_64-linux-gtk2.tgz, see http://pgopher.chm.bris.ac.uk/Help/installlinux.htm for further instructions.
 You should be ready to use the program
- 2. There is also a very detailed online help on the website (which you can use in case the help function installed on your computer does not work).
- 3. Download the .zip files with the material for the tutorial from the shared repository, the link will follow.

References

Western, Colin M. 2017. "PGOPHER: A Program for Simulating Rotational, Vibrational and Electronic Spectra." *Journal of Quantitative Spectroscopy and Radiative Transfer* 186 (January): 221–42. https://doi.org/10.1016/j.jqsrt.2016.04.010.