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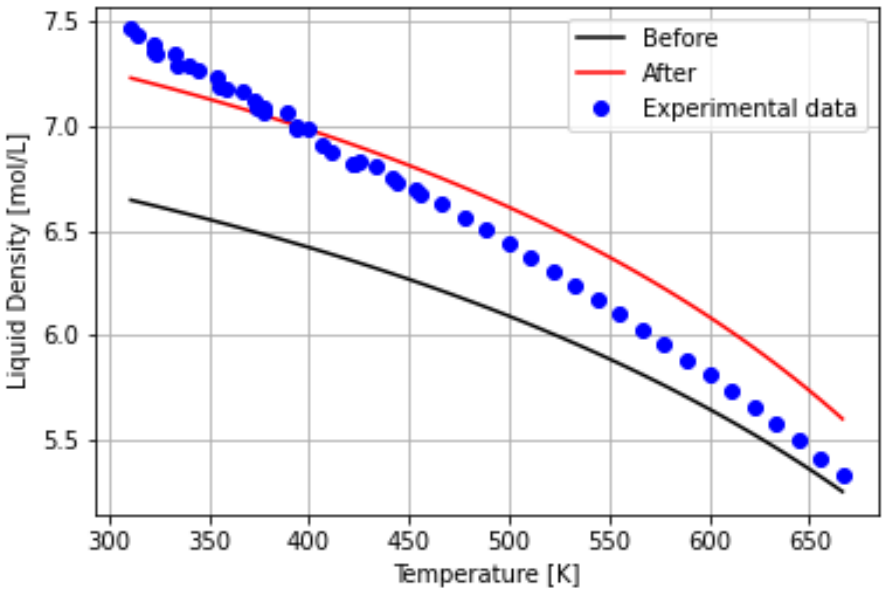
PyThermo

Thermodynamic Phase Equilibria Modelling in Python

User Guide, Edition 1

Software version, 1.0.2



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June 25, 2021

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Published by: DTU, CERE, Building 229, 2800 Kgs. Lyngby Denmark

https://www.cere.dtu.dk/

Acknowledgements

John Towne, MSc - For developing a Python package with optimization algorithms, including Particle Swarm and Nelder Mead algorithms.

Contents

1 Introduction to PyThermo

PyThermo is a Python package dedicated to performing thermodynamic modelling on phase equilibria. Additionally, the package contains functions for performing pure component parameterization

Currently the models include the following equations of state:

- CPA
- SRK
- PR
- PC-SAFT
- ePC-SAFT
- eCPA

The package is available on PyPi at
https://pypi.org/project/pythermo/

The GitHub page for Pythermo is found on the following URL:
https://github.com/olisimdan/PyThermo

2 Installation of Python and Packages

2.1 Python

Using PyThermo requires Python version 3.8.3 or higher. The newest releases of Python may be found on the official website:
https://www.python.org/
However, we recommend installing Python by installing Anaconda, which include the latest version of Python in its installation.

2.2 Anaconda

It is strongly adviced to use Anaconda when using PyThermo, please refer to the following URL or Anaconda installation:
https://www.anaconda.com/products/individual

2.3 Installing Integrated Development Environment (IDE)

The authors of PyThermo recommend using Visual Studio Code as the Python IDE, for an installation guide refer to the following URL:
https://code.visualstudio.com/Download

When Visual Studio Code is installed, a Python extension must be installed. In order to do this, refer to the following URL:
https://marketplace.visualstudio.com/items?itemName=ms-python.python

Since a Python interpreter has already been installed through Anaconda, you can safely ignore that part of the Python extension guide.

2.4 Installation of PyThermo

Once the above mentioned prerequisites have been met (Anaconda installed and IDE installed), it is time to install the PyThermo package. There are two ways of doing this. The first and easy way, is via *pip*

1. Open Anaconda Prompt.
2. Type `pip install pythermo` in the window.
3. Press enter, and let the installation commence.

If the above approach fails, please follow this approach

1. Head to https://github.com/olisimdan/PyThermo and download the entire directory.
2. Save the directory somewhere on your computer.

3. Open Anaconda Prompt.
4. Type `cd <package directory>`. As an example, `cd C:/Users/username/Desktop/PyThermo`, and press enter.
5. Type ”python setup.py install”
6. Press enter, and let the installation commence.

And this point PyThermo should be successfully installed, along with necessary packages.

3 Jupyter Notebook

Jupyter notebook is used as an interactive tool to test and learn PyThermo.

3.1 How to open Jupyter Notebook

First, open Anaconda Prompt (this won't work in the regular Command Prompt, unless it has been properly set up - so for ease of use, utilize Anaconda Prompt).

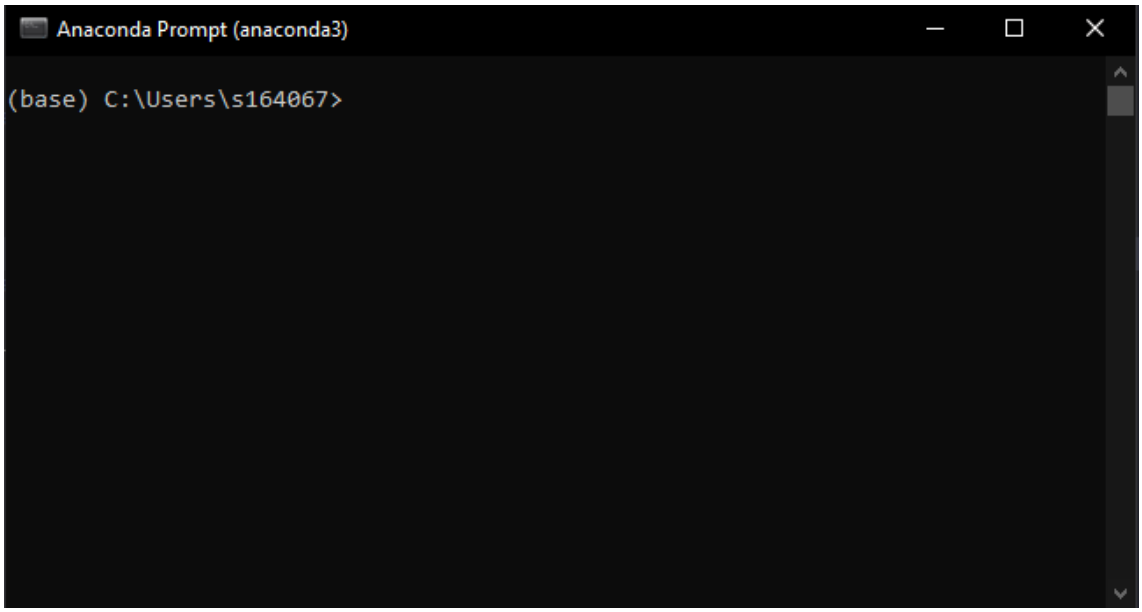

Figure 1: Anaconda Prompt - Empty

Type "jupyter notebook", all lower case in the terminal.

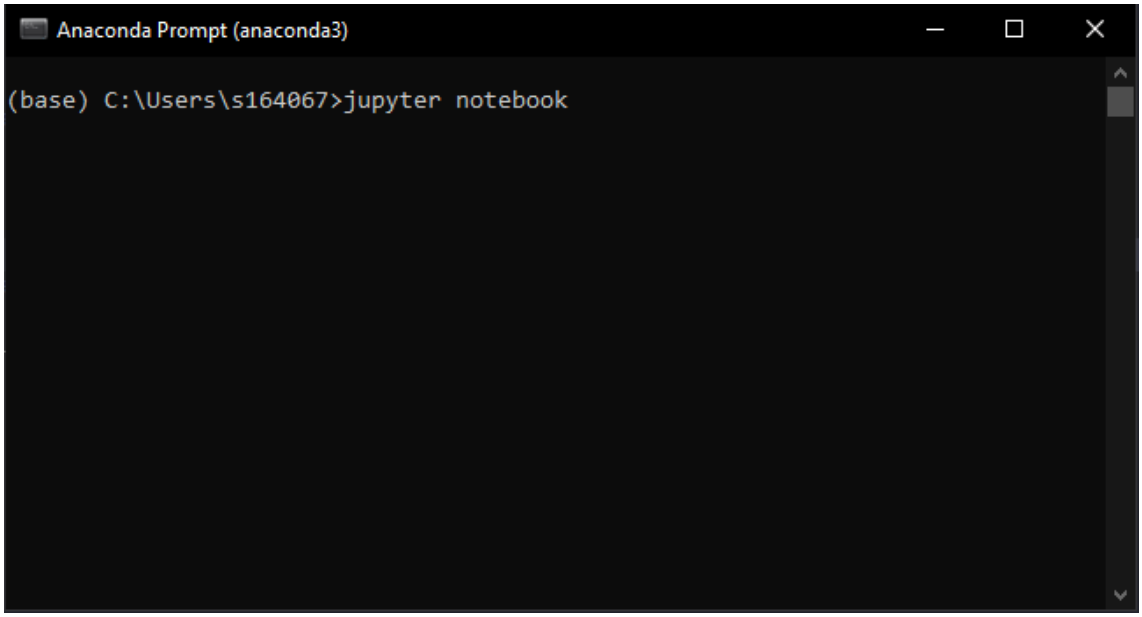

Figure 2: Anaconda Prompt - Write "jupyter notebook"

A bunch of text will appear in the terminal. Near the bottom, there will be a URL that you may copy and insert into the browser address bar.

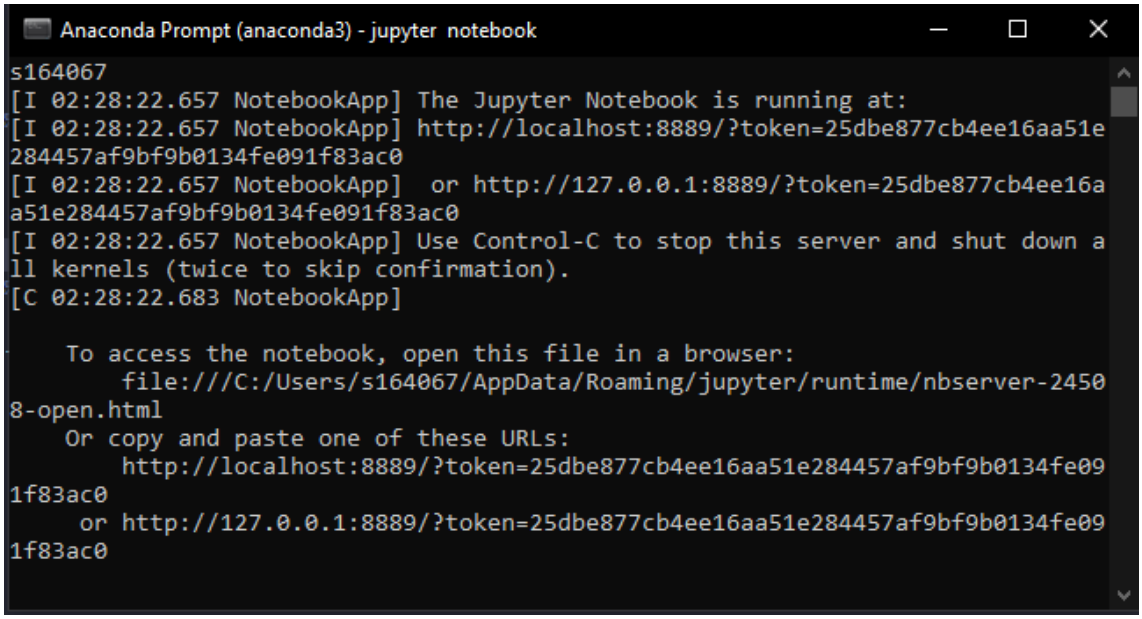

Figure 3: Anaconda Prompt - Press enter

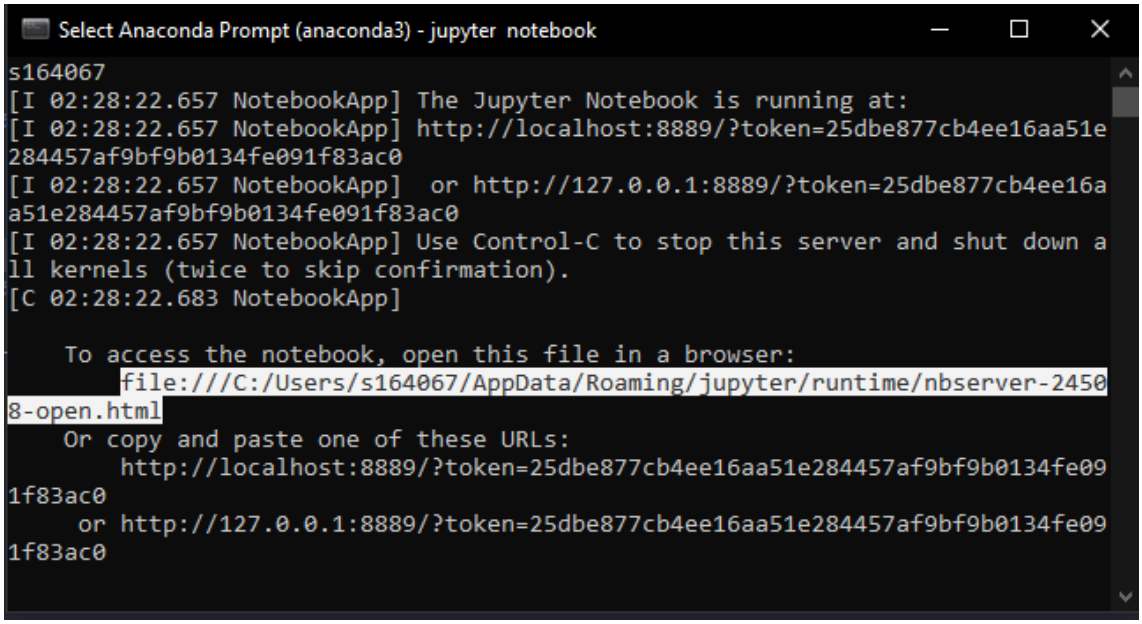

Figure 4: Anaconda Prompt - Copy URL

Once the URL has been pasted into the browser address bar, you will be met by the following screen.

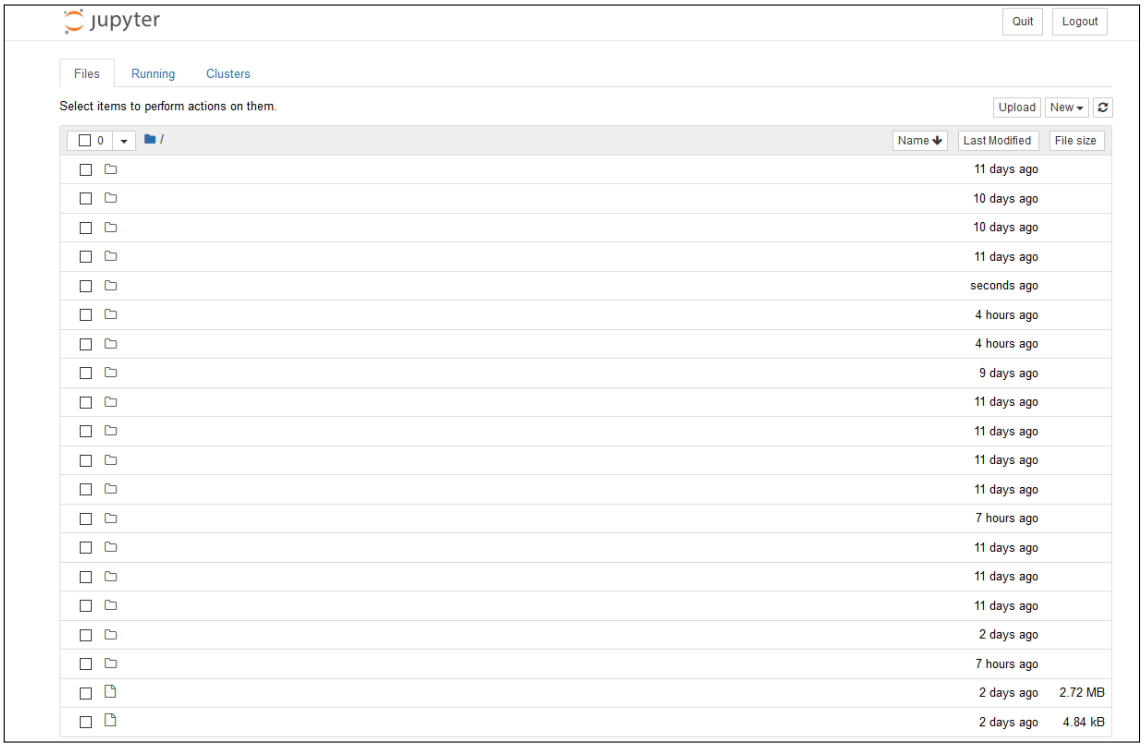

Figure 5: Directory explorer in Jupyter Notebook.

From here we may navigate to the Jupyter Notebooks.

3.2 How to use Jupyter Notebook

From the browser window opened (see previous section), head to ”tests” folder, and then ”jupyter_notebooks” folder. From here all Jupyter Notebooks may be opened by pressing them.

3.3 Jupyter Notebooks for PyThermo

Below is a list of the six Jupyter Notebooks offered in this Python package.

- Preparing Thermodynamic Calculations
- Performing Thermodynamic Calculations
- Comparison Functions
- Parameter Optimization
- Uncertainty Analysis
- Advanced Parameter Estimation

4 PyThermo Syntax

The Python documentation for the PyTherm module may be found by following the following procedure.

1. Head to the folder containing the downloaded files.
2. Open the directory called ”docs”
3. Open the shortcut called ”Python Documentation”. Any browser may be used.

Below you will see an example from the documentation page.

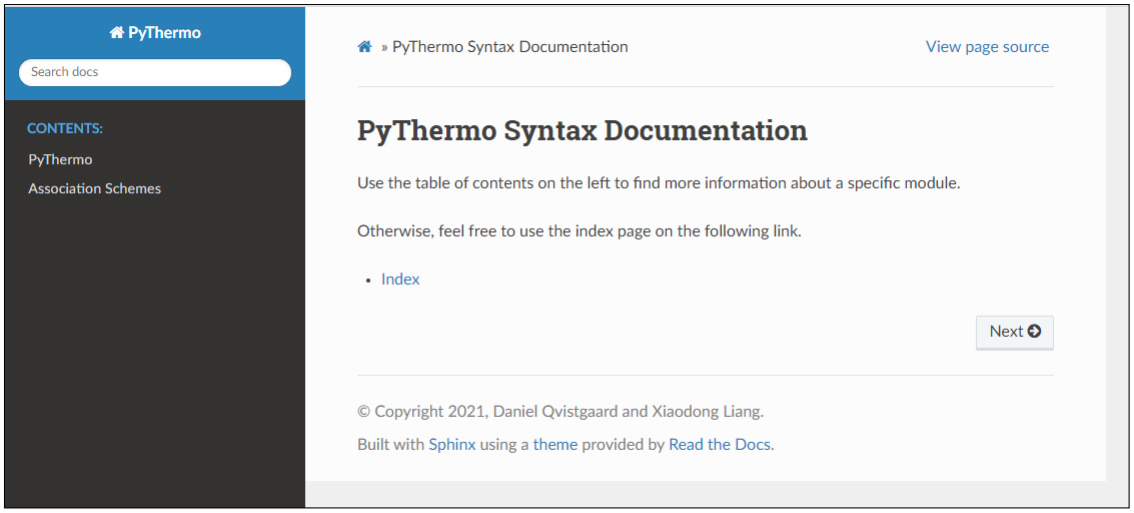

Figure 6: Screenshot of the documentation page

From the front page the user may navigate to one of two tabs on the left hand side of the screen. The tab called ”PyThermo” contains Python documentation for the use of this package. See the screenshow below:

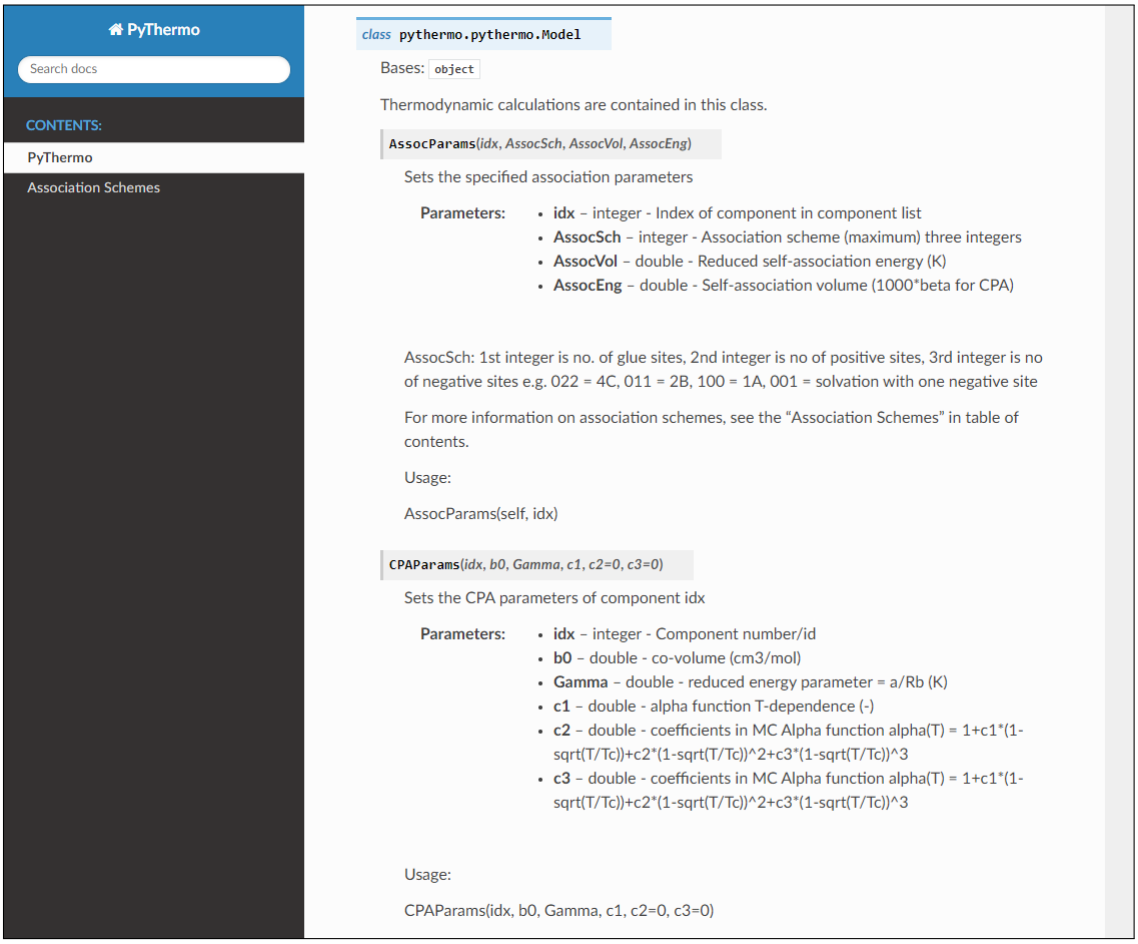

Figure 7: Screenshot of the documentation page

The second tab available on the left hand side is is called ”Association Schemes”, and is a short list of known association schemes and their corresponding integers for defining the scheme, which is used in the CPA model. See the screenshot below:

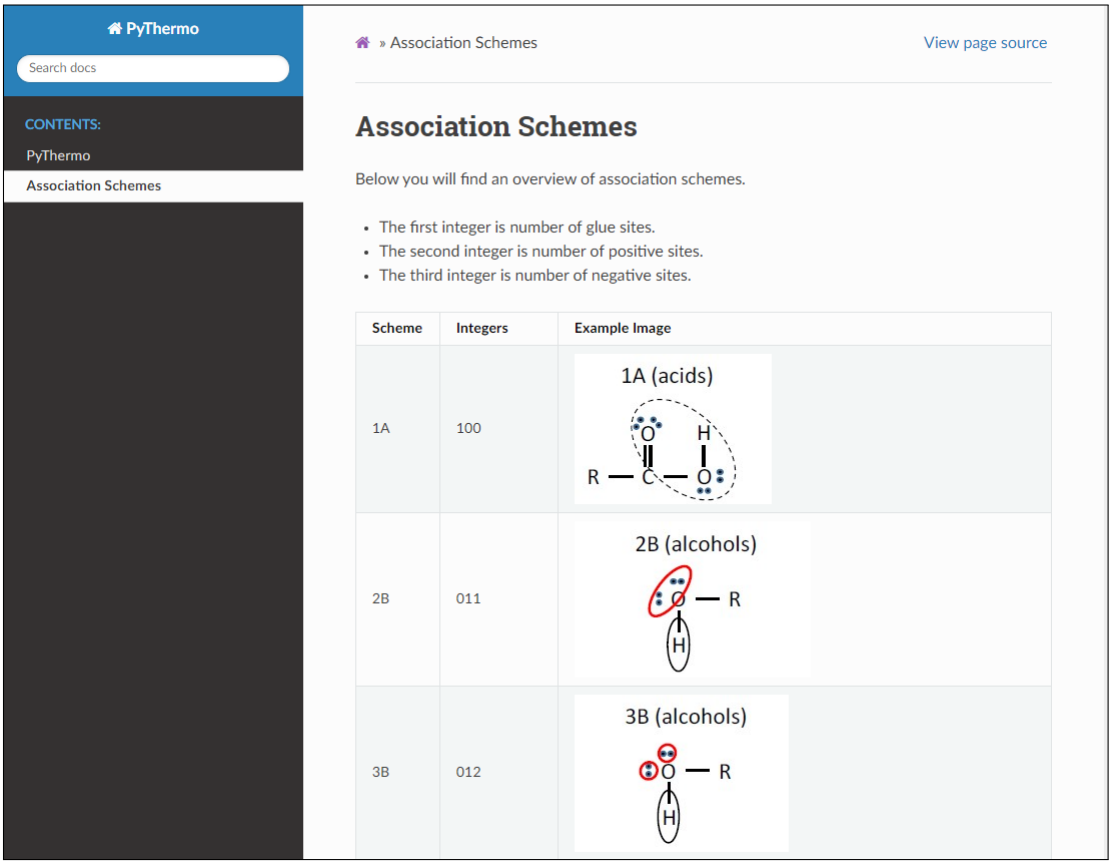

Figure 8: Screenshot of the documentation page