

CH40208: TOPICS IN COMPUTATIONAL CHEMISTRY

GOOD CODING PRACTICE AND TESTING

WRITING READABLE CODE

- ▶ Python is a very **readable** programming language, once you understand the logic
- ▶ We can leverage this by using it to write readable code
 - ▶ Using sensible variable names
 - ▶ Being consistent
 - ▶ Being concise, but clear
 - ▶ Using conventions

SOME UNREADABLE CODE

```
# Ugly, hard to read code
s = ['H', 'Ca', 'Fe', 'Hg', 'Br', 'Xe']
m = [13.99, 1115, 1811, 234.321, 265.8, 161.4]
b = [20.271, 1757, 3134, 629.88, 332, 165.051]
for k, d in enumerate(range(0, len(s))):
    if m[d] < 273.15 and b[d] >= 273.15:
        print(s[d])
        print("This element is a liquid and not a
solid or a gas at standard temperature and
pressure.")
```

SOME UNREADABLE CODE

- ▶ Problems with this code
 - ▶ What are `s`, `m`, and `b`?
 - ▶ `enumerate(range(0, len(s)))` will create two numbers that are the same
 - ▶ The purpose of the `if` statement line is not clear
 - ▶ The final line is very long and hard to read

SOME RULES FOR READABILITY

- ▶ The Python community has some guidelines to improve code readability; known as PEP 8
- ▶ You can take this further, for example good variable names
- ▶ **Be aware**; the final assessment will include marks linked to clarity and readability of code

COMMENTS

- ▶ Commenting code is one of the easiest ways to improve clarity of purpose
- ▶ Any line starting with a `#` is a comment and will not be run
- ▶ The purpose of comments is to explain the why the code does something, not what the code is doing
- ▶ This is a **pointless** comment

```
sum = 1
# Iterate from 1 to 5
for i in range(1, 5):
    sum *= i
```

DOCSTRINGS

- ▶ Docstrings are a special type of comment that describe the function, arguments and returned of a function
- ▶ These are particularly useful as automated programs can be used to generate formatted documentation from them
- ▶ There are many *styles* of doctoring but we will use the NumPy style

DOCSTRINGS

```
import numpy as np

def pH(H):
    """Determine the pH for a given H+ concentration

    Parameters
    -----
    H: float
        Concentration of H+ (or H3O+) in solution

    Returns
    -----
    float
        The pH value
    """
    return np.log10(H)
```


DOCSTRINGS



DEMO

TESTING

- ▶ We are not perfect, and neither is the code we write
- ▶ Therefore we need a way to check that our code does what we think it does
- ▶ This is achieved with testing
- ▶ Testing (in Python) could be the topic for a whole lecture course, however we will show the basics

TESTING

- ▶ Tests are run at a function level
- ▶ Therefore to write useful tests functions should be as small as possible
- ▶ Some functions will require just one test
- ▶ Others (depending on the flow control in the function) may require many

TESTING



DEMO

TEST DRIVEN DEVELOPMENT

- ▶ TDD is a methodology in computer programming where a set of tests are written as the spec for the code
- ▶ **Then** the code is written so that it can pass the tests
- ▶ This has become particularly popular on large, collaborative projects

PROBLEM

- ▶ Apply the test driven development methodology
- ▶ Download the zip file from Moodle and write the code (as functions in the Jupyter Notebook) that will pass the tests defined in the `test_functions.py` module