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

▸ Using relevant comments

▸ Including descriptive docstrings for functions

▸ Attempt to keep line length relatively short

▸ Write modular code; put short functions into module

SOME UNREADABLE CODE

```python
# 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 d in 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`?

   ▸ The purpose of the `if` statement line is not clear

   ▸ The final line is very long and hard to read

▸ **Be aware**; the final assessment will include marks linked to the aspects mentioned previously

SOME RULES FOR READABILITY

▶ **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 why the code does something, not what the code is doing

▸ This is a **pointless** comment

```python
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 docstring but we will use the Google style

DOCSTRINGS

```python
import numpy as np

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

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


    Returns:
        float: The pH value
    """
    return np.log10(conc_h)
```
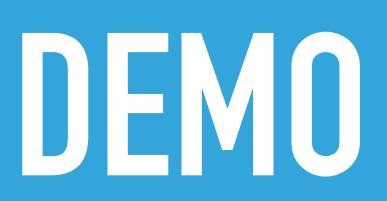
DOCSTRINGS

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 should do

▸ 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 module) that will pass the tests defined in the `test.ipynb` notebook