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

```
# 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 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 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